



90th Annual Meeting

of the International Association of
Applied Mathematics and Mechanics

February 18-22, 2019

Vienna, Austria

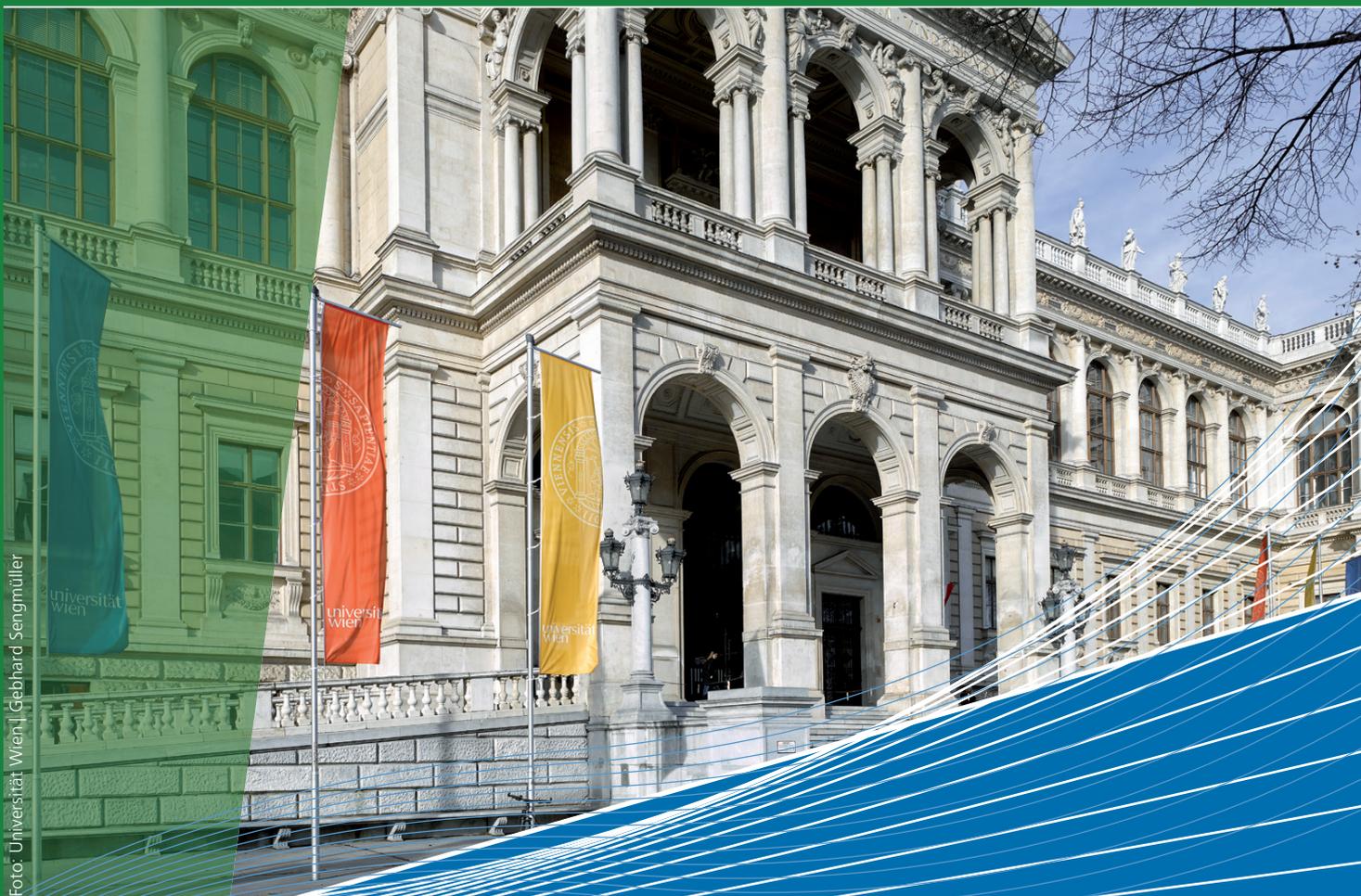


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Book of Abstracts



**Book of Abstracts of the
90th Annual Meeting of the International Association of Applied
Mathematics and Mechanics (GAMM 2019)**
February 18-22, 2019, Vienna, Austria

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Prandtl Memorial Lecture and Plenary Lectures

Ludwig Prandtl Memorial Lecture 2019

Date: February 18, 2019

14:00-15:00

Room: Audimax, streaming to BIG HS

Finite-size Lagrangian coherent structures

Hendrik C. Kuhlmann (*TU Wien, Austria*)

When a small particle is transported in an incompressible flow, which is steady in some frame of reference, the particle can be attracted to a periodic orbit or to a more complex attractor. Usually, such an attractor is caused by inertia forces on the particle, which rely on the density mismatch between particle and fluid. However, attractors can also be caused by repulsive forces from a boundary acting on the particle due to its finite size. The mechanism leading to particle-motion attractors by particle-boundary interaction is discussed and typical examples are presented. While the mechanism acts on a single particle, many or even all particles of a dilute suspension can cluster on or near the single-particle attractor. If the attractor is periodic or quasi-periodic the resulting particulate structure is called finite-size Lagrangian coherent structure. In systems with tangentially moving boundaries finite-size coherent structures can form very rapidly, because their creation relies on repeated particle-boundary interactions, the period of which scales with the characteristic time of the flow. The effect leading to finite-size coherent structures may find application in sorting particles by their size in microsystems when other methods cannot be applied.

Plenary Lecture 1

Date: February 18, 2019

15:00-16:00

Room: Audimax, streaming to BIG HS

Composable solvers in PETSc/Tao: from linear systems and differential equations to optimization

Barry Smith (*Argonne National Laboratory, Chicago, United States of America*)

Many of the most popular scalable linear solvers can be obtained mathematically as the composition of one or more simple (even trivial) solvers. The same holds true for nonlinear solvers, as well as for many ODE integrators and optimization algorithms. The key is the structure of the compositions selected to combine the simple solvers. I will discuss, within the context of the PETSc solver package, a variety of such compositions and how they can be leveraged to develop clear code that implements the algorithms with a great deal of code reuse.

Plenary Lecture 2

Date: February 19, 2019

11:00-12:00

Room: Audimax, streaming to BIG HS

Direct methods for camera-based 3D reconstruction & SLAM

Daniel Cremers (*Technische Universität München, Germany*)

The reconstruction of the 3D world from images is among the central challenges in computer vision. Starting in the 2000s, researchers have pioneered algorithms which can reconstruct camera motion and sparse feature-points in real-time. In my talk, I will introduce direct methods for camera tracking and 3D reconstruction which do not require feature point estimation, which exploit all available input data and which recover dense or semi-dense geometry rather than sparse point clouds. They lead to a drastic boost in precision and robustness. Furthermore, I will showcase some applications ranging from 3D photography and 3D television to autonomous navigation.

Plenary Lecture 3

Date: February 19, 2019

12:00-13:00

Room: Audimax, streaming to BIG HS

PDE constrained Bayesian inference: when numerics meets statistics

Robert Scheichl (*Universität Heidelberg, Germany*)

Advances in modern science and engineering almost always involve a combination of experimental research and numerical simulation. To better understand, predict or design complex physical or engineering systems, mathematical modelling, e.g. via partial differential equations (PDEs), has become an irreplaceable component. Weather and climate prediction, the design of modern aircraft and energy materials, or the certification of nuclear waste repositories are only a few examples. Numerical methods for PDEs and their implementations on high performance computers have reached a level of sophistication that allows the numerical simulation of ever more complex, heterogeneous, nonlinear processes. Many openly available PDE software packages exist. However, model parameters and initial/boundary conditions are typically only partially available or measurable and those measurements are often indirect and/or noisy. On the other hand, statistical methods for inverse problems that allow to infer distributions of unknown or uncertain parameters given (noisy) measurements of the system have also reached a very high level of sophistication. In particular, Bayesian techniques are well understood and developed, such as the gold-standard Metropolis-Hastings MCMC or filtering techniques, but also variational approaches. The application of Bayesian inference to complex PDE constrained problems is still a hugely challenging task though. This is partly due to their high computational complexity (i.e. cost versus accuracy), but also due to the typically very high dimensional parameter domain in PDE constrained applications. To overcome this challenge requires a concerted effort of statisticians, numerical mathematicians and application scientists, which has spawned the new scientific research area of Uncertainty Quantification (UQ). In this talk, I will present a number of examples from my research where classical ideas from numerical mathematics are used to increase the efficiency of Bayesian statistical methods for PDE problems, in particular hierarchical

approaches such as multilevel Monte Carlo, or low-rank matrix and tensor approximations and the use of Hessian (Newton) information in sampling methods.

Plenary Lecture 4

Date: February 21, 2019

11:00-12:00

Room: Audimax, streaming to BIG HS

Modeling and simulation of transport processes at fluid interfaces

Dieter Bothe (*Technical University of Darmstadt, Germany*)

Besides the already rich hydrodynamics of two-phase flows, additional transport and transfer processes like heat or mass transfer, Marangoni effects as well as phase change phenomena are of utmost importance in numerous applications with fluid interfaces. In the present talk, main emphasis will be put on mass transfer processes at clean and contaminated interfaces. The talk surveys recent developments for simulating several small-scale phenomena occurring at moving, deformable fluid interfaces with applications to liquid films, droplets and gas bubbles. The underlying models are based on sharp-interface continuum physics with different levels of complexity concerning physico-chemical interface properties, where special attention is devoted to thermodynamic consistency. The numerical solution of the resulting models is built on different approaches such as the Volume of Fluid method or Arbitrary-Lagrangian-Eulerian Interface Tracking. These approaches include the accurate treatment of interfacial jump conditions, thin concentration boundary layers and the solution of interfacial PDEs accounting for surface active agents.

Plenary Lecture 5

Date: February 21, 2019

12:00-13:00

Room: Audimax, streaming to BIG HS

Mechanical metamaterials

Dennis M. Kochmann (*ETH Zürich, Switzerland, California Institute of Technology, USA*)

Mechanical metamaterials are man-made solids with a carefully engineered small-scale architecture to result in beneficial effective mechanical properties. What started with acoustic metamaterials for controlling linear waves has recently been extended into various directions, including e.g. metamaterials with optimized stiffness, strength, fracture toughness, damping, or nonlinear wave propagation for a myriad of engineering applications. Being a playground for experimentalists, theoreticians and modelers alike, this area at the diffuse interface between materials and structures is rapidly expanding and combines many concepts of mechanics and applied mathematics - from homogenization and effective property extraction to the accurate constitutive modeling and fabrication of multiscale materials systems. Unlike e.g. in the creation of composite materials and alloys, the design space here resides at significantly larger, structural scales and therefore admits manipulation of the metamaterial's microstructure with relative ease (e.g., the effective properties of periodic truss networks depend on the topology and geometry of the truss unit cell, whose limitations are only set by fabrication constraints). Besides experimental challenges associated with descending to ever-smaller scales, theoretical and computational challenges have called for methods to describe the effective, macroscale response of such heterogeneous multiscale architectures. We will survey recent progress made on those fronts while also highlighting selected

open challenges and opportunities. Particular focus will be on, among others, the mechanics of lightweight truss networks and their modeling by discrete, continuum and discrete-to-continuum coupling techniques, and the nonlinear dynamic response of soft metamaterials which allows to mimic inelastic material phenomena at the structural level.

Plenary Lecture 6

Date: February 21, 2019

16:30-17:30

Room: Audimax, streaming to BIG HS

A fluid mechanic's analysis of the tea-cup singularity

Dwight Barkley (*University of Warwick, United Kingdom*)

In 1926 Einstein published a short paper explaining the meandering of rivers. He famously began the paper by discussing the secondary flow generated in a stirred tea cup – the flow now widely known to be responsible for the collection of tea leave at the center of a stirred cup of tea. In 2014, Luo and Hou presented detailed numerical evidence of a finite-time singularity in a rotating, incompressible, inviscid flow. The key driving mechanism of that singularity is the secondary tea-cup flow. The present work is not aimed at proving the existence of a singularity in this flow, nor is it aimed at generating more highly resolved numerical evidence for the singularity than already exists. Rather, I will assume that the flow simulated by Luo and Hou genuinely develops a singularity. My goal is to understand, from a fluid-mechanics perspective, why.

Plenary Lecture 7

Date: February 22, 2019

11:00-12:00

Room: Audimax, streaming to BIG HS

History and recent developments of energy-momentum schemes

Peter Betsch (*KIT Karlsruhe, Germany*)

Energy-Momentum (EM) schemes belong to the class of structure-preserving numerical discretization techniques. This specific discretization approach aims at the preservation of main structural properties of the underlying continuous system. Originally EM schemes were developed in the context of nonlinear elastodynamics to provide enhanced numerical stability and robustness in the iterative solution procedure. In particular, the seminal paper by Simo and Tarnow (J.C. Simo, N. Tarnow, The Discrete Energy-Momentum Method. Conserving Algorithms for Nonlinear Elastodynamics, ZAMP, 43, 757-792, 1992) sparked numerous works on the design of EM schemes for nonlinear structural dynamics and elastodynamics. EM schemes are capable to exactly reproduce major balance laws in the discrete setting, independent of the mesh size (in space and time). In nonlinear elastodynamics the focus is on the balance laws for energy and angular momentum. Due to their success in nonlinear applications EM schemes have been further developed to cover more elaborate problems such as large deformation contact and flexible multibody dynamics. In recent years EM schemes have been extended to coupled field problems such as large deformation thermo-mechanics and electro-mechanics. This extension gives rise to the notion of Energy-Momentum-Entropy (EME) schemes that typically provide enhanced numerical stability and physical reliability of the numerical results. The talk will address the development of EM schemes from their origins in nonlinear elastodynamics to their extension to EME schemes for coupled nonlinear field problems.

Plenary Lecture 8

Date: February 22, 2019

12:00-13:00

Room: Audimax, streaming to BIG HS

Towards unified hierarchical modeling of hard and soft biological tissues

Christian Hellmich (*Vienna University of Technology, Austria*)

Traditionally, the realms of hard and soft tissue biomechanics are strictly separated: hard tissue biomechanics is typically based on elasto-plastic or elasto-damage formulations in the small strain regime, while soft tissue biomechanics has its roots in hyperelastic rubber modeling. Both of these two traditional approaches face the challenge of highly scattering material parameters, which rarely allow for reliable predictions of untested situations. In the hard tissue realm, this challenge has been met with the advent of engineering micromechanics in the early 2000s. Key ingredients of this success were the hierarchical sequencing of traditional homogenization schemes such as two-phase Mori-Tanaka and self-consistent schemes, the extension from two-phase to multi-phase systems, and the consideration of eigenstrains and their upscaling characteristics, which paved the way towards a unified vision of bone multiscale biomechanics [1], encompassing poro-elasticity [2], poro-plasticity [3,4], and creep [5]; all based on a few “universal” mechanical properties of bone’s elementary components: collagen, hydroxyapatite, and water. Can this success be repeated also for soft tissues? The lecture will give an affirmative answer, based on recently developed theoretical tools [6] allowing for the modeling of load-induced changes in the tissue micro-morphology, as it evolves under large strains at different observational levels.

References:

- [1] J Theor Biol 244, 597-620, 2007
- [2] Ultrasonics 54, 1251-1269, 2014
- [3] J Theor Biol 260, 230-252, 2009
- [4] Int J Plast 91, 238-267, 2017
- [5] Comp Meth Biomech Biomed Eng 17, 48-63, 2014
- [6] ZAMM DOI: 10.1002/zamm.201700360, 2018

Minisymposia

MS1 | Mathematical modeling, analysis and simulation of drug distribution for efficient pharmacotherapy

Date: February 19, 2019 14:00-16:00
Room: HS 34
Organiser: Jurjen Duintjer Tebben (*University of Prague, Czech Republic*)
Elfriede Friedmann (*University of Heidelberg, Germany*)

Predicting drug disposition and metabolism in breast tumours

Amy Barber (*University of Surrey, United Kingdom*) 14:00
Nick Plant (*University of Leeds, United Kingdom*)

Breast cancer is the most prevalent cancer among women worldwide, with nearly 1.5 million diagnoses in worldwide per year. Despite the development of a range of therapeutics, for use both in isolation and as combinations, the mortality rate for breast cancer has remained stubbornly high. Reasons underlying this include the highly heterogeneous molecular underpinning of breast cancer, and the fact that drug distribution through tumours is still poorly understood. A better prediction of how drugs distribute through tumours and the cellular responses to the local drug concentration is critical for the development of personalised therapies. To this end, we have used a range of both in vitro and in silico approaches we have explored the generation of multi-scale, multi-formalism models to predict breast cancer tumours to therapeutic drug combinations.

Using literature searches and in vitro experimentation, we characterised breast cancer cell lines for a range of parameters (doubling time, metabolite production and consumption, and response to therapeutic agents). These data were used to parameterise an in silico model integrating the Recon2 genome-scale metabolic network with gene regulatory networks for oestrogen and progesterone receptors, using our quasi-steady-state Petri net approach within the MultiFormalism Interaction Network Simulator (MuFINS). This generic model ‘personalised’, using a congruency approach to overlay transcriptomic data for both cell lines (MCF7, MDA-MB-231) and 2,000 patients (Metabric dataset). Personalised models were explored to identify potential metabolic vulnerabilities. These predictions were confirmed in vitro, demonstrating proof-of-concept for this network-targeting paradigm to identify novel drug combinations.

Drug distribution through tumours is complex, meaning it is not a simple matter to extrapolate from in vitro experiments to in vivo response. This is particularly true when trying to optimise the concentration of more than one drug, as is the case with combination therapy. Using both discrete, compartment-based and continuum, PDE-based models drug disposition across a tumour was simulated and then used as an input to the previously described metabolic models. This allows prediction of how cells within different regions of a tumour (and thus exposed to different concentrations of drugs, oxygen and nutrients) will respond to drug exposure.

The work motivates further examination of how to further integrate these models into a true multi-scale, multi-formalism model that represents multiple levels of biological organisation. Such models, when complete should aid our understanding of the context-specific optimisation of drug therapy.

An introduction into current mathematical drug distribution models from the pharmacologic point of view

Petr Pavek (*Charles University Prague, Czech Republic*) 14:30
Jurjen Duintjer Tebbens (*Charles University Prague, Czech Republic*)

The aim of this talk is to provide a critical overview of the most current types of mathematical models used in modern pharmacologic research to predict concentration-time-profiles and effect of administered drugs, with emphasis on drugs binding to nuclear receptors. Important challenges, from the pharmacologic point of view, for the current models are pointed out. These include the need to cope with high inter-donor variability of physiological parameters, the need to refine basic models through incorporating long-term effects with repeated dosing and through taking into account drug-drug interactions when considering promiscuous receptors. These may lead to more complex feedback-loops that are often understood rather poorly. Benefits of including spatial resolution are planned to be addressed as well as issues related to the highly desired but also highly non-trivial extrapolation of rodent *invivo* models to reliable human *invivo* simulations.

On conservative and unconditionally positivity preserving numerical methods

Andreas Meister (*University Kassel, Germany*)

15:00

Stefan Kopecz (*University Kassel, Germany*)

For the solution of positive and conservative production-destruction systems we introduce modified Patankar-Runge-Kutta (MPRK) schemes. They adapt explicit Runge-Kutta schemes in a way to ensure positivity and conservation irrespective of the time step size. Within the talk we introduce a general definition of MPRK schemes and present a thorough investigation of necessary as well as sufficient conditions to derive first, second and third order accurate MPRK schemes. The theoretical results will be confirmed by numerical experiments in which MPRK schemes are applied to solve non-stiff and stiff systems of ordinary differential equations.

Mathematical modelling of intracellular protein dynamics: the importance of the spatial organisation of an eukaryotic cell

Zuzanna Szymanska (*Polish Academy of Sciences, Poland, University of Warsaw, Poland*)

15:30

Martin Parisot (*Inria - ANGE, France*)

Mirosław Lachowicz (*University of Warsaw, Poland*)

Weronika Wronowska (*University of Warsaw, Poland*)

We propose a spatio-temporal model of intracellular protein dynamics, i.e. protein and mRNA production and transport inside a cell, that takes into account active transport along microtubules in the cytoplasm as well as diffusion and is able to reproduce the oscillatory changes in protein concentration observed in many experimental data. On the basis of numerical simulations, we formulate a new hypothesis that the oscillatory dynamics is caused by the mRNA active transport along microtubules from the nucleus to distant locations. The proposed model is generic, built with a focus on the possibility of its adaptation to specific signalling pathways. We extend our previous model of heat shock response pathway, that is crucial in cells adaptation to stress conditions caused by hyperthermia or some cytotoxic drugs, to take into account the spatial organisation of a eukaryotic cell.

MS2 | Topology optimization of structures considering elaborate constraints and variables

Date: February 19, 2019 14:00-16:00
Room: BIG HS
Organiser: Thomas Vietor (*Technische Universität Braunschweig, Germany*)
Axel Schumacher (*University of Wuppertal, Germany*)
Sierk Fiebig (*Volkswagen AG, Germany*)

Compilation of activities to extend the standard topology optimization procedures for real mechanical problems

Thomas Vietor (*TU Braunschweig, Germany*) 14:00
Sierk Fiebig (*Volkswagen AG, Germany*)
Axel Schumacher (*Bergische Universität Wuppertal, Germany*)

The current methods for topology optimization of mechanical structures initially divide the design space into many small (sub-)domains and decide for each of these domains depending on defined criteria whether there should be material or not. This can lead to interpretable structures. The currently available topology optimization program systems are still very limited in their applicability. Often, small deviations from the standard formulation, the minimization of compliance while considering a volume or mass constraint already leads to difficulties and the possibility of misinterpretations.

This contribution gives answers to the question, which extensions are necessary in the future so that the topology optimization of mechanical structures can be used even more. The contribution shows practice-relevant extensions and completely new approaches regarding the definition of the optimization problem:

- Integration of production constraints: Every focused manufacturing process must be integrated so intensively that the designer no longer has to make any major changes after the optimization. In addition to the simulation of the manufacturing process, manufacturing rules must be integrated. For example, work on the integration of casting and the integration of deep drawing are presented.
- Automation of the process from CAE to CAD: Better smoothing algorithms and automatic creation of CAD elements are needed. For this purpose, current solutions are shown.
- If the problems are structurally more complex, completely new approaches must be developed. Here we have to mention the optimizations considering the acoustics and crash behavior. For example, methods for topology optimization of crash structures are presented.
- Robustness aspects must be included in the optimization.

The paper allows an overview of existing application domains and objects for an extension of the applicability of topology optimization for future areas.

Topology optimization for real industrial design problems

Ming Zhou (*Altair Engineering Inc, United States of America*) 14:20
Raphael Fleury (*Altair Engineering Inc, United States of America*)
Fabian Fuerle (*Altair Engineering Inc, United States of America*)
Linlin Zhao (*Altair Engineering Inc, United States of America*)

Application of topology optimization has grown significantly in the last two decades. Twenty years ago, there were just a handful of commercial software available. Today all major CAE vendors offer such solutions, and there are many more solutions provided by smaller companies

and startups. Topology optimization has also been the most active sub-field of structural optimization for the last two decades. It should, however, be pointed out that most research and software solutions are limited in scope relative to real industrial design problems. For real engineering design problems, it is essential to include comprehensive coverage of responses including static responses such as stress, displacements and dynamic responses such as frequency, vibration etc. Additionally, it is important to consider variety of manufacturing constraints such as minimum and maximum member sizes, casting, extrusion etc. In recent years additive manufacturing and topology optimization have emerged as a powerful combination for design innovation. Manufacturing aspects specific to AM should also be addressed. These include overhang control and lattice structure design. Another important aspect for application is design interpretation and geometry creation. This paper will provide a comprehensive treatment on how to formulate real world design problem, and how to create efficient industrial-grade solutions. Applications will be shown to demonstrate impact of topology optimization to design innovation across broad industries.

Application of topology optimization in automotive industry

Lothar Harzheim (*Opel Automobile GmbH, Germany*)

14:40

Today, topology optimization modules are an integral part of almost any FEM software based on linear analysis. Even if the practical application often involves more difficulties than described in the brochures, topology optimization is an effective tool with very high optimization potential. In contrast to shape or sizing optimization, topology optimization helps to determine the optimized global features of components such as cross sections, locations of reinforcements or number and arrangement of ribs inside an open profile. Even if the resulting new design has to be fine-tuned in many cases using shape and/or sizing optimization, it turns out that the largest portion of the improvement is mostly reached by the selection of an optimized topology.

Due to the tendency of the optimizer to create hollow proposals with holes, the interpretation of a design proposal and the transformation into a producible design can sometimes be very difficult if no manufacturing constraints are included in topology optimization. In particular, this is true for the optimization of cast parts. It will be demonstrated, how the quality of the proposal can be increased drastically by using auxiliary models or by applying manufacturing constraints and the resulting effects are discussed in detail.

The application of topology optimization in the nonlinear area, in particular for crash, is the real challenge today. The ESL-method (Equivalent Static Load-method) is one way to solve such a nonlinear optimization task because it provides a procedure to extract linear auxiliary load cases from a nonlinear analysis enabling a linear static optimization. Hence, all optimization types such as sizing, shape, topography and topology optimization can be applied. However, there are some issues to be solved such as how to define responses such as section forces and HIC-values, which are defined in the nonlinear system only and are not available in the linear analysis. Especially, for topography and topology optimization there are additional issues, which cannot be solved by using commercial ESL-codes. For this reason an in-house ESL-code has been developed at Opel. An overview above the current status, results and drawbacks and, finally, an outlook for the future development will be given.

Form finding by shape optimization and vertex morphing

Kai-Uwe Bletzinger (*Technische Universität München, Germany*)

15:00

The proper parameterization of structural shape which is suitable for creating, analyzing, finding and optimizing structural form is a great challenge. The demand for large design spaces with large and very large numbers of design parameters is continuously increasing. However, there is

a conflict with the requirements for flexible and intuitive application and the robustness of the numerical model. Also, design parameterization applying standard CAD tools which are based on explicitly formulated splines appears to be most cumbersome even for numbers of parameters which are not larger than 100. In contrast, the Vertex Morphing Method (VMM) directly uses the discretization nodes or vertices as design parameters to morph the structural shape by applying filters. VMM overcomes all numerical burdens and is most intuitive and easy to be used. The actual presentation will show that filtering is equivalent to the implicit definition of standard spline models which makes VMM most interesting and compatible to standard design procedures. Filters as design morphing tools are most effective to define and to control the local and global shape properties. In the context of form finding and shape optimization filters are applied to the shape sensitivity fields as the generator of the design update towards the optimum. Impressive form finding and optimization applications in the fields of CSD and CFD with problem sizes up to 3.5 million shape design parameters can easily be handled by this technique and will be presented.

References

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- [2] M. Hojjat, E. Stavropoulou, and K.-U. Bletzinger, "The vertex morphing method for node-based shape optimization," Computer Methods in Applied Mechanics and Engineering, vol. 268, pp. 494-513, 2014.
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Meta-modelling of the missing link between the analytical Topological Derivative equations and sensitivities for the optimization of crash loaded structures

Katrin Weider (*Bergische Universität Wuppertal, Germany*)

15:20

Axel Schumacher (*Bergische Universität Wuppertal, Germany*)

The Topological Derivative (TD) is the sensitivity of a functional for the introduction of an infinitesimal hole into the mechanical body. For linear elasticity problems in structural mechanics the TD is known in a closed analytical form for various functionals. The formulation of the Topological Derivative is based on the adjoint state approach and the known analytical form of the stress distribution around circular cavities in linear elasticity. That allows the calculation of an easily evaluable analytical form for the sensitivity. Because the stress distribution around circular cavities for arbitrary nonlinear material models is not known as an analytical solution, the above-mentioned analytical form is limited to Hooke's law.

For the sensitivity analysis of crash loaded structures, where time dependency and geometrical and material nonlinearities appear, the TD was recently derived also in analytical formulas [1] - with the exception of the stress and strain distribution on the boundary of the fictitious hole. This stays in the unsolvable integral formulas.

In this contribution, a microscale investigation, that replaces the analytical integral formulas with meta-models is presented. Corresponding to the analytical procedure, a microcell Finite Element model with a circular hole in a planar shell is loaded under two perpendicular forces and two perpendicular moments, that represent the loading in the macroscale initial boundary value problem. Various combinations of these forces and moment provide the sample points for the meta-model of the TD.

Using the Finite Element Method for the solution of the macro-scale crash problem, the Topological Derivative can be requested from the meta-model and the sensitivity of the design space can

be derived pointwise. For functionals, that cope with crash relevant requirements, a discussion about different meta-model techniques will be illustrated with an academic example.

Reference

- [1] Weider, K., Schumacher, A.: “Adjoint Method for Topological Derivatives for optimization tasks with material and geometrical nonlinearities”, EngOpt 2018 Proceedings of the 6th International Conference on Engineering Optimization, 2019, Springer Nature Switzerland AG

Optimization of structure-borne sound propagation using structural intensity

Sebastian Rothe (*Technische Universität Braunschweig, Germany*)

15:40

Sabine Christine Langer (*Technische Universität Braunschweig, Germany*)

Reducing noise in mobile applications such as cars, aircraft and trains is a major challenge for today’s engineers. In most cases, sound sources and radiating structures are locally separated. The airborne sound field is a result of the excitation and the transfer through the mechanical system. The resulting structure-borne sound is propagated on transfer paths and finally radiated through plate-like structures. Therefore, the structure-borne sound energy should already be efficiently damped on the way of propagation.

The structural intensity (STI) is a complex vectorial quantity that represents the flow of sound energy in the structure. The real part of STI, can identify areas with a high absorption of structure-borne sound. These areas should correlate with high damping in the structure, e.g. areas with additional applied damping measures. If the damping is homogeneously distributed, a uniform distribution of structure-borne sound energy should be the objective in order to make optimum use of the material damping. The energy flow can be influenced by introducing structural changes. With the help of the direction information and the quantitative value of the STI, the position of such structural changes can be optimized.

In this paper, an optimization procedure is investigated, with which a homogenization of the structure-borne sound flow is aimed. Numerical studies on generic structures are carried out. The STI for a homogeneous and an inhomogeneously damped plate is calculated and specifically influenced by various measures (e.g. point masses, beads). The aim is the targeted guidance of sound in areas of high damping or the uniform distribution in the structure in order to reduce the mean velocity in a defined frequency range.

MS3 | Research software and -data: How to ensure replicability, reproducibility, and reusability

Date: February 19, 2019 14:00-16:00
Room: HS 50
Organiser: Jörg Fehr (*University of Stuttgart, Germany*)
Christian Himpe (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Sustainable research software

Andreas Zeller (*Saarland University, Germany*) 14:00

Large amounts of software are created in science for scientific purposes. How can we make this software sustainable, such that it can be run, integrated, and extended by others? In this talk, I show some of the most important principles to give software a long and impactful life.

Sustainable development of research software

Jörg Fehr (*University of Stuttgart, Germany*) 14:20
Christian Himpe (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Stephan Rave (*WWU Münster, Germany*)
Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Research software is one of the main corner stones of modern scientific progress. In many areas of the sciences first numerical evidence is sought in computer experiments, also called in-silico labs, before entering the wet-lab. Today chemical reactions are designed on computers before getting verified in the lab, process controls are adapted in elaborate computer experiments before getting applied in the real world and new materials emerge from computer-based optimization. Yet, the education of the code-developing researchers and the existence of the maintenance infrastructure for the corresponding software is often still falling far behind the needs of the scientific endeavors. On a day-by-day basis, this leads to archaic and error-prone methods in the design and implementation of scientific software with low degrees of reusability.

Our contribution analyses the situation and gives recommendations that aim to improve the situation for both small projects like a basic program used in a thesis, and larger packages like a work groups "in-house"-code or research communities software tool.

Integrating publication, software and data in simulation sciences

Bernd Flemisch (*University of Stuttgart, Germany*) 14:40
Timo Koch (*University of Stuttgart, Germany*)
Martin Schneider (*University of Stuttgart, Germany*)

While the process of publishing scientific findings in form of journal articles can be considered to be mature, this doesn't hold in general for the supplementary material associated with such an article. In simulation sciences, this material may consist of the software that has been used to produce the results that are presented in the article as well as research data such as simulation results or experimental measurements used for model validation. Although methods and tools for developing and publishing research software as well as for managing research data already

exist and are under continuous development, standardized workflows for their employment in simulation sciences are still in their infancy. Especially the integration of the three components publication, software and data poses special challenges.

In this talk, we present our efforts for making our publications transparent and reproducible by accompanying them with the associated software, data and metadata. Concerning the software, these efforts are based on employing our open-source porous-media simulator DuMux. Within a project called DuMux-Pub, we provide for each publication a Docker container storing the complete software stack that is necessary to run the simulations producing the corresponding results. Concerning the research data, we present the workflow that is being developed currently within the Collaborative Research Centre SFB 1313 and the SimTech Cluster of Excellence EXC 2075, together with the university library and the computing center in Stuttgart. As a frontend for uploading, sharing, publishing and archiving data, we use Dataverse, an open-source research data repository software. The integration of publication, software and data is one of the main goals of the project "Sustainable infrastructure for the improved usability and archivability of research software" that has been granted recently by the DFG.

FAIR principles for research software and data in the area of computer-based simulation

Sibylle Hermann (*University Stuttgart, Germany*)

15:00

The FAIR Data Principles define guiding principles of how to archive and publish research results like software and data in a way to make them reusable for oneself as well as others. Therefore, the research results should be Findable, Accessible, Interoperable and Reusable (FAIR). The key to achieving accessibility and sustainability is the description of data in the form of metadata: Metadata should be written in standardized, machine-readable language and using defined vocabulary. At the same time, it has to include search criteria as well as descriptions on data-provenance. Persistent identifiers like DOIs give access to software and data regardless of their actual storage location and they link the data and metadata to each other. Open protocols and standards guarantee interoperability. These protocols and standards for data formats and metadata have to be discussed and developed within scientific communities. Different initiatives try to establish the idea of being FAIR. The GoFair-Initiative, for example is an international bottom-up movement that encourages, the standardized development of the global Internet of FAIR Data and Services. They support and coordinate implementation networks. They work on concrete and practical solutions for culture change, training and technical solutions for the implementation of the FAIR Data Principles in the scientific community. An approach for the engineering sciences has been made in the Conference of European Schools for Advanced Engineering Education and Research (CESAER), Task Force Open Science (TFOS). The aim is to identify the best practices in engineering and provide guidance through principles for FAIR and secure data. To develop those guidelines TFOS collected case studies of research data. Their aim is to understand the views and needs of scientists from engineering disciplines on data management and to improve the support of FAIR engineering data in infrastructures and repositories. In the area of computer-based simulations there is a lot of potential for the replicability, reproducibility and reuse of data and software. Metadata standards for data (like DataCite) or Software (like CodeMeta) are already in existence and can be used as a basis for the description of the inputs and results of computer-based simulations. Persistent identifiers like DOIs are available for implementations. In addition the FAIR Data Principles give a framework to help scientific communities establish rules for their research needs. Infrastructure, as libraries, can only offer technical support and advice; whether the rules are applied and prevail depends on the individual researcher.

Devising a new fluid dynamics solver based on generic mathematical software libraries

Martin Kronbichler (*Technical University Munich, Germany*)

15:20

In my talk, I will present our work on a new solver for incompressible fluid flow, targeting the simulation of transitional and turbulent flows. Time integration is done by a dual splitting method based on the BDF family. For the spatial discretization, high-order discontinuous Galerkin methods are used. To render high polynomial degrees efficient, matrix-free evaluation of discrete operators rather than sparse matrix algebra is essential. This setup goes against common practice in PDE software design because the implementation of finite element components must be integrated into the linear solvers, rather than outsourcing all linear algebra to external packages. Nonetheless, generic software design is possible by providing mathematical descriptions of discretized finite element and discontinuous Galerkin operators in an abstract way. I will present the design in the generic library deal.II, which requires the application code to only provide an implementation of the operation in quadrature points of cell and face integrals. All the integration as well as loop over the mesh can be provided by the library, including the MPI ghost communication and parallelization strategies.

In my talk, I will discuss that this setup allows to combine performance close to the capabilities of the computer hardware, while allowing the application solver to be relatively compact. Such a design is of key importance for making the solver applicable to a wide range of application, but also helps the ingredients for the incompressible Navier-Stokes equations. For example, a stable discretization with discontinuous Galerkin methods for under-resolved high-Reynolds number flows requires the velocity to be exactly divergence free, which can be either realized by so-called Raviart-Thomas velocity spaces and discontinuous pressures or by suitable penalty terms on the velocity divergence and the continuity of the normal component of velocity over element boundaries. With our solver, these auxiliary operators can be implemented efficiently. I will evaluate the impact of these terms on the overall performance and characterize the overall solver performance.

An automated performance evaluation framework for the Ginkgo software ecosystem

Hartwig Anzt (*Karlsruhe Institute of Technology, Germany*)

15:40

We present a framework that automates the process of testing and monitoring the performance of software libraries. Integrating this component into an ecosystem enables sustainable software development as a community effort via a web application for interactively evaluating the performance of individual software components. The performance evaluation tool is based exclusively on web technologies, which removes the burden of downloading performance data or installing additional software. The framework is currently integrated into the Ginkgo sparse linear operator library, but allows for easy extension to cover other software projects. This enables the painless comparison of different high performance computing libraries.

MS4 | Coupled problems in rotating machinery

Date: February 19, 2019 14:00-16:00
Room: HS 21
Organiser: Wolfgang Seemann (*Karlsruhe Institute of Technology (KIT), Germany*)
Aydin Boyaci (*ABB AG, Germany*)
Dominik Kern (*Chemnitz University of Technology, Germany*)

A mixed variational-based dynamic simulation method for fiber-reinforced continua in non-isothermal rotordynamical systems

Michael Groß (*TU Chemnitz, Germany*) 14:00
Julian Dietzsch (*TU Chemnitz, Germany*)
Chris Rübiger (*TU Chemnitz, Germany*)

Three-dimensional woven carbon-fiber reinforced polymers (3D-CFRP) are being increasingly used for blades in rotordynamical systems as turbine fans and wind turbines as well as disc brake rotors. These light-weight materials allow for lower rotational masses while maintaining stiffness and improving heat conduction properties. This leads in turbine fans to higher possible rotational speeds, and allows for longer and thus more efficient blades in wind turbines. Thereby, the direction-dependent heat conduction allows for a more efficient cooling in high temperature environments.

By using dynamic mixed finite-element methods, these materials can be simulated as anisotropic continua with non-isothermal behaviour in the matrix as well as the fiber material. On the other hand, the rotordynamical systems in which these 3D-CFRP are applied are often formulated by variational approaches. Simulation techniques building on these approaches are preferable. Therefore, we present a novel dynamic mixed finite-element method which is variational-based, and therefore capable to simulate these materials in rotordynamical variational formulations. This dynamic mixed finite-element method preserves each basic balance law emanating from the variational principle exact in a discrete setting. This leads to more physically-consistent results concerning the thermo-mechanical coupling effects. By using independent fields for the deformation of the matrix and the fibers, we also avoid unphysical locking effects. We demonstrate this physically-consistent simulation behaviour by using dynamic simulations of a turbine rotor, a disc brake rotor and a rotating heat-pipe subject to thermal and mechanical loads.

Coupled effects of the rotor support at vibration based monitoring

Samuel Krügel (*Technical University Munich, Germany, Siemens AG Corporate Technology, Germany*) 14:20
Johannes Maierhofer (*Technical University Munich, Germany*)
Christian Wagner (*Technical University Munich, Germany*)
Thomas Thümmel (*Technical University Munich, Germany*)
Daniel Jean Rixen (*Technical University Munich, Germany*)

Vibration based monitoring of rotating machinery by measuring at the outside housing gains in importance for industry. Especially when considering integrated sensor systems, due to wireless transmission capacity, external measurement points are mandatory. Even though, correlating access is comfortable and requirements for sensor mounting as well as for protective casing are lower than at bearing seats, coupling effects of rotor and housing are striking. Particularly, within the scope of monitoring various rotor fault types, as described in [1], structural dynamics of the

entire system must be well known. One parameter affecting rotor fault force transfer to sensor positions is the kind of support. Within this contribution, we show the effect of the orthotropic-elastic supported rotor [2] on unbalance monitoring. Therefore, we present an example, used as industrial application for cooling of drive systems. The considered blower was evaluated at different defect states and assembled with radially distributed, external accelerometers to answer two questions:

- May a suspected unbalance be verified by measuring at the outside housing at different operating conditions?
- Which coupling problems between rotor and measurement position due to orthotropic-elastic rotor support may occur and how can they be solved?

Thereby, we figured out, that the suspected unbalance can be verified by measurements, but only between global resonance frequencies of the application, because they superimpose the acquired signals in mode shape directions, initially evoked by unbalance excitation. Furthermore, we demonstrate the direction reversion of measured unbalance signals due to phase shift of mode shape correlating measurement directions at resonance frequencies. Thus, forward and backward whirl expresses themselves within the rotational frequency but does not restrict unbalance monitoring, provided that the global modes are well known.

References

- [1] Thümmel, T.; Roßner, M.; Ulbrich, H., and Rixen, D., Unterscheidung verschiedener Fehlerarten beim modellbasierten Monitoring, in H. Ecker, H. Irretier, R. Liebichand, R. Markert, R. Nordmann, and J. Strackeljan, editors, 11. Internationale Tagung Schwingungen in Rotierenden Maschinen (SIRM), Magdeburg, Germany, 2015.
- [2] R. Gasch, R. Nordmann, and H. Pfützner, Rotordynamik (Springer-Verlag, Berlin Heidelberg, 2006), chap. 5. DOI:10.1007/3-540-33884-5

First critical speed determination of a rotor via low-speed measurements

Horst Ecker (*Vienna University of Technology, Austria*)

14:40

Johann Kogler (*Vienna University of Technology, Austria*)

Knowing the critical speed of an actual rotor system is very important for several reasons. For an actual rotating machinery it may define the maximum speed to avoid undue stress or even damage to the rotor. Numerical calculations may give answers, but only if the system parameters are known with sufficient accuracy. Since the operation of a weakly damped rotor at or near a critical speed can be too dangerous, vibration data may only be collected at speeds within reasonable distance of the yet unknown critical speed.

Recently, Virgin, Knight and Plaut [1] proposed a method to evaluate low-speed vibration measurement data such that the actual critical speed can be predicted accurately. The basic idea of this new method is to generate FRF-like functions (aka Southwell-plots) that can be analysed such that a prediction of the critical speed is possible.

In this contribution, the authors have tested this new method on a rotor test rig with a vertical shaft. The arrangement was similar to a Jeffcott-rotor, but altogether four ball bearings were attached to hold the very flexible and weakly damped shaft. Emphasis was put on running the experiments under real word conditions, i.e. imperfections like initial shaft bow, misaligned bearings and bearing anisotropy were present in the system. Operation parameters, as for example bearing temperature, were changed and their influence was studied.

The evaluation of the proposed method did show that this method did give very good results. The accuracy obtained was typically within a few percent of the actual critical speed. The imperfections of the rotor system in use did not have a destructive influence on the method. However, the quality of the results did depend in some cases heavily on the selection of the

measurement points used for the extrapolation routine. As one may expect, the accuracy was reduced, when unfavourable measurement points were selected. From this experimental work, guidelines can be deduced how to apply this technique such that high-fidelity predictions of the first critical speed of a rotor can be made, based on low-speed measurements.

[1] L .N. Virgin, J .D. Knight, R .H .Plaut (2016), A New Method for Predicting Critical Speeds in Rotordynamics, *Journal of Engineering for Gas Turbines and Power*, 138 (2), 022504.

Non-linear vibrations in rotor systems with floating ring bearings induced by fluid structure interactions

Elmar Woschke (*Otto-von-Guericke-Universität Magdeburg, Germany*) 15:00

Steffen Nitzschke (*Otto-von-Guericke-Universität Magdeburg, Germany*)

Christian Daniel (*Otto-von-Guericke-Universität Magdeburg, Germany*)

For a sustainable analysis of the rotor dynamic behaviour of hydrodynamically supported systems the nonlinear effects resulting from the journal bearings have to be considered. This can take place in various manners always with regard to the application and the task of the analysis. For transient loads and operational conditions usual assumption of analytical solutions of the governing Reynolds equation has restricted accuracy concerning the non-linear force laws which depend on position and velocity of the bearing partners. Thus numerical approaches have to be used. At this point the interaction between the hydrodynamics and rotor dynamics can be enlarged by additional influencing field problems like thermodynamics (energy equation and thermal behaviour of the surrounding structure) or structural dynamics (local and or global elastic deformations due to acting forces or even thermal loads). As a result for specific systems like turbochargers, crank drives or gas turbines the coupled effects have to be analysed concerning their influences on each other. Hence, adapted simulation methods have to be used. Furthermore the necessary level of detail for the description of the nonlinearity to assure an appropriate result for the vibration in an adequate time is rather unclear. Especially effects resulting from cavitation are often neglected in transient analyses. Thus, in this contribution an extended and time efficient approach for the numerical consideration of cavitation in journal bearings and floating ring bearings is presented and the differences to common approaches are studied for different conditions and rotor types. The results are validated with measurements and compared concerning their advantages and disadvantages with other model assumption. Additionally the mentioned effects of structural dynamics are considered in various forms as well as different types of thermal behaviour, always with respect to accuracy and the necessary computation time.

Numerical analysis of fluid-film-cavitation on rotordynamic vibration and stability behavior

Huaxin Dong (*TU Darmstadt, Germany*) 15:20

Gerrit Nowald (*TU Darmstadt, Germany*)

Daixing Lu (*TU Darmstadt, Germany*)

Bernhard Schweizer (*TU Darmstadt, Germany*)

The dynamic vibration and stability behavior of a rotor supported in journal bearings is investigated. In the lubricating film of a hydrodynamic bearing, different cavitation phenomena may occur. Cavitation in hydrodynamic bearings is most commonly caused by surrounding air, which is sucked into the bearing gap or by outgassing of dissolved gases. Cavitation effects should be considered in order to precisely analyze the performance of rotor/bearing systems.

Numerous approaches have been proposed to treat cavitation using appropriate boundary conditions in the pressure equation, which is applied to calculate the hydrodynamic pressure distribution in the bearing gap (Reynolds fluid film equation). These approaches are generally divided

into two types: non mass-conserving and mass-conserving cavitation models. In this paper, a mass-conserving cavitation model based on a two-phase approach (lubricant/air mixture) is applied. For the two-phase model, a relationship has to be defined that describes the dependency between pressure and density of the mixture. Different pressure/density models are presented and discussed.

Numerical run-up simulations are performed to study the stability of rotor/bearing systems incorporating different cavitation models. The numerical model for the rotor/bearing system consists of a multibody model for the rotor and a finite element model for the fluid film. Both models are coupled by a co-simulation approach. The different cavitation models are compared. The influence of the cavitation model and the cavitation parameters on the stability behavior of the rotor/bearing system is analyzed. The cavitation approaches are also compared with respect to accuracy and efficiency.

Some aspects of the impact of using foil bearings on rotor dynamics

Benyebka Bou-Said (*INSA Lyon, France*)

15:40

The aeronautical designers of turbo shaft engines have, at all times, rapidly dealt with very strong requirements of weight. Consequently, these designers focussed towards the increase in the specific power involving the reduction in the size of the machines and the increase number of revolutions. In ranges of 30000 with more than 200 000 rotation rpm, an aerodynamic assistance seems well adapted compared to the traditional technological elements which cannot answer given requirements, as for example the lifetime. Thus the air bearings received in these last decades a considerable attention and find increasingly many applications whenever raised speeds, weak loads and a high degree of accuracy are necessary. The aeronautical applications relate to mainly auxiliary power units (APU) and air conditioning machines. Gas lubrication makes possible the limitation of the power loss by fluid friction. In these mechanisms the rotor is supported by foil bearings lubricated with surrounding air. Between the shaft and the housing, which are not coaxial, there is a radial clearance and therefore a possible effect of aerodynamic lift in the convergent when the shaft is in rotation. The film of air in the convergent is in the order of 3 - 10 μm and the pressure in the film is sufficient to support the weight of the rotor and all radial external forces. The forces generated in the film allow the rotor to remain in its equilibrium position, in permanent regime. These last decades numerous models of foil bearings have been developed. Today, the limits of these models are obvious particularly for the understanding of non linear behaviors of the system rotor/bearing and for the quantification of its energy dissipation. It is essential for future developments to control instabilities linked to the running conditions of these bearings. The objective of this study is to provide a modeling of the bearing as close as possible to the real behavior. Thanks to a variational approach and FEM, the flexible structure is modeled as a thin structure in large displacement subjected to compressible fluid pressure, thermally insulated. Both laminar and turbulent flow situations have been investigated. The structure deformation is obtained with an Updated Lagrangian Method and we take into account the internal dry friction using the Coulomb's law. Thanks to a frequency analysis, we observe a higher magnitude response of subsynchronous frequencies as the whirl. This study is completed with experimental comparisons.

MS5 | Input-to-state stability of distributed parameter systems

Date: February 19, 2019

14:00-16:00

Room: HS 01

Organiser: Andrii Mironchenko (*University of Passau, Germany*)

Felix Schwenninger (*University of Hamburg, Germany*)

ISS and ISS-Lyapunov functions: an introductory overview

Lars Grüne (*University of Bayreuth, Germany*)

14:00

In this talk we give an introductory overview on input-to-state stability (ISS) - a stability concept for dynamical systems with inputs introduced by Eduardo Sontag in 1989 - and its relation to ISS Lyapunov functions.

We will start from the observation that globally asymptotically stable finite dimensional linear systems have a "built in" robustness against additive perturbations which is in general lost for nonlinear dynamics and - most important for this minisymposium - for infinite dimensional state space. The ISS concept recovers this robustness property for nonlinear or infinite dimensional systems.

We explain how this robustness can be characterized by so called ISS Lyapunov functions and discuss different types of such functions which are useful for different classes of systems.

Input-to-state stability for nonlinearly boundary-controlled port-Hamiltonian systems

Jochen Schmid (*University of Würzburg, Germany*)

14:20

Hans Zwart (*University of Twente, The Netherlands*)

In this talk, we are concerned with the stabilization of linear port-Hamiltonian systems on an interval (a, b) (for instance, vibrating strings or beams) in the presence of external disturbances. In order to achieve stabilization we couple the system to a nonlinear dynamic boundary controller whose output is allowed to be corrupted by an external disturbance before it is fed back into the system. We first establish the well-posedness of the resulting nonlinear closed-loop system and then present two input-to-state stability results for the closed-loop system (with input being the external disturbance): for a special class of nonlinear controllers, we obtain uniform input-to-state stability and for a more general class of nonlinear controllers, we obtain weak input-to-stability (in fact, even convergence of all solutions to zero).

Optimal stabilization of flows by value function approximations

Tobias Breiten (*University of Graz, Austria*)

14:40

Karl Kunisch (*University of Graz, Austria*)

Laurent Pfeiffer (*University of Graz, Austria*)

The optimal control design of flows described by the Navier-Stokes equations has been and still is an active area of research. For problems with an infinite time horizon, i.e. stabilization problems, methods are often based on Riccati equations arising for the linearized system. The resulting feedback laws can be interpreted as an approximation of the value function to the lowest order. Higher order approximations are tied to differentiability properties of the value function. As presented in the talk, in an appropriate functional analytic setup, the value function can be shown to be smooth. This yields a way of computing higher order feedback laws without solving the Hamilton-Jacobi-Bellman equation.

Strong input-to-state stability for infinite-dimensional linear systems

Robert Nabiullin (*University of Wuppertal, Germany*)

15:00

Felix Schwenninger (*University of Hamburg, Germany*)

For linear systems the notion of input-to-state stability implies exponential stability of the undisturbed system. In many applications this assumption is too strong but one is still interested in stability properties with respect to inputs. This leads to the notion of strong input-to-state stability. In this talk the relation between the strong versions of input-to-state stability and integral input-to-state stability is studied for linear boundary control systems. We show that strong input-to-state stability with respect to inputs in an Orlicz space is a sufficient condition for a system to be strongly integral input-to-state stable for bounded inputs. If the undisturbed system is exponentially stable both stability notions are equivalent. In general, the converse is not true.

Stability and well-posedness for non-autonomous port-Hamiltonian systems

Björn Augner (*Technische Universität Darmstadt, Deutschland*)

15:20

Hafida Laasri (*Bergische Universität Wuppertal, Deutschland*)

We study the non-autonomous version of an infinite-dimensional port-Hamiltonian system. Employing abstract results on evolution families we provide sufficient conditions for which the non-autonomous port-Hamiltonian system is well-posed and the corresponding evolution family is exponentially stable.

ISS small gain theorems for spatially invariant systems

Fabian Wirth (*University of Passau, Germany*)

15:40

Spatially invariant systems are a class of distributed parameter systems obtained by coupling finitely dimensional systems according to a graph structure so that the resulting system has an interesting symmetry group. Under the assumption that each of the subsystems is input-to-state stable we study the question under which conditions on the coupling structure and the system gains input-to-state stability of the overall system is guaranteed.

For benign symmetry groups we show that the resulting small-gain condition is essentially finite-dimensional. In the case of linear gains the conditions reduce to results already available in the literature. The construction of ISS Lyapunov functions will be discussed.

Young Researchers' Minisymposia

YRM1 | Modeling and control of Port-Hamiltonian systems

Date: February 18, 2019 16:30-18:30
Room: HS 31
Organiser: Robert Altmann (*University of Augsburg, Germany*)
Philipp Schulze (*Technische Universität Berlin, Germany*)

Dimension- and complexity-reduction for nonlinear partial differential port-Hamiltonian equations preserving an energy interpretation

Björn Liljegren-Sailer (*Universität Trier, Germany*) 16:30
Nicole Marheineke (*Universität Trier, Germany*)

The development of approximation schemes for evolution problems, which take into account fundamental underlying physical principles, has been an active field of research in the last decades. There exists a large body of problem-specific space- and time-discretization schemes. Unified frameworks for larger classes of systems are, however, less developed. Moreover, for model-order and complexity-reduction structure-preserving schemes is a rather open topic, especially for nonlinear systems. One very promising structured modeling framework of evolution problems is the port-Hamiltonian framework. In this contribution we take up the modeling paradigm behind port-Hamiltonian systems and present a variational framework for the construction of online-efficient reduced models for a large class of nonlinear partial differential equations. The focus lies on the preservation of dissipative relations, or respective discrete counterparts. All approximation steps are taken into account, which are discretization, projection-based model-order-reduction, and complexity-reduction of the nonlinearities to avoid the so called lifting bottleneck.

Trajectory control of an elastic manipulator based on the discretized port-Hamiltonian model

Mei Wang (*Technische Universität München, Germany*) 17:10
Paul Kotyczka (*Technische Universität München, Germany*)

This contribution deals with the trajectory control of an elastic robot arm based on the discretized port-Hamiltonian (pH) model. In order to follow a given planar movement for the beam tip as well as to reduce the occurring oscillations, we consider the two-degrees-of-freedom control scheme. The developed control concept is implemented and tested on a laboratory manipulator, which was built at our institute.

The flexible beam is fixed on a rigid hub and driven horizontally by a brushless DC motor with a harmonic drive gear. The beam is modeled as a Timoshenko beam. We apply the geometric pseudo-spectral method to discretize the Timoshenko beam model, which preserves structural properties in the lumped-parameter model, in particular the power balance. The two subsystems are interconnected to an overall pH model. In order to use the finite-dimensional model in real time for observer-based state feedback control, the system order is reduced by means of structure-preserving model reduction.

The structure of the reduced pH beam model is exploited for inversion-based feedforward control so that the beam tip follows the given trajectory. The nominal motor torque is computed taking into account the motor dynamics. The friction in the drive unit highly depends on the operating conditions, e.g. temperature. The motor angle, the motor speed and the angular velocity of the beam tip are available for measurement. In order to estimate the remaining states and to

compensate the unknown friction, an observer with a disturbance model is applied for the state variable difference. Experimental results with an elastic robot arm illustrate the applicability of the approach by high-fidelity tracking of the reference trajectory and suppression of residual oscillations.

Numerical approximation of heat transfer on heterogenous media

Tobias Scheuermann (*Technische Universität München, Germany*)

17:50

Paul Kotyczka (*Technische Universität München, Germany*)

Distributed parameter systems are locally described by partial differential (PDE) equations. These PDEs are the basis for numerical methods to simulate the underlying physical system. Well-known examples are finite element methods, finite difference methods and finite volume methods (FVM). A special form of FVM is the cell method [5, 6]. It utilizes the correlation between physical variables and geometric objects [2]. These objects and their relations to each other can be described by a generalized graph, a so-called k-complex. The discrete balance laws can be described exactly with the incidence matrices of the k-complex and its dual. Together with the approximation of the constitutive laws, a given port-Hamiltonian form of the system equations is preserved in the discretized model [4, 3].

In a homogeneous medium with the assumption of continuously varying material parameters, a grid with desired resolution is generated to define control volumes. An approach to deal with heterogeneous media is to find surrogate parameters [1] which depend on the material and the structure of the media.

This work uses another approach: Instead of a generated grid, the structure of the medium itself is used for discretization. We consider an open cell metallic foam and analyse in a first step the transport of heat. The topological and geometrical data, defines the primal complex on which the balance of internal energy is evaluated. A dual k-complex is constructed, on which discrete thermodynamic driving forces are defined. Together with the approximation of the constitutive laws, a discrete model is obtained, that retains the structure of the local conservation laws.

Literature

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- [5] Enzo Tonti. A direct discrete formulation of field laws: the cell method. *Computer Modeling in Engineering and Sciences*, 2(2):237-258, 01 2001.
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YRM2 | Recent advances in Galerkin methods based on polytopal meshes

Date: February 18, 2019 16:30-18:30
Room: BIG HS
Organiser: Lorenzo Mascotto (*University of Vienna, Austria*)
Steffen Weißer (*Saarland University, Germany*)

Discontinuous Galerkin methods for the biharmonic problem on polygonal and polyhedral meshes

Zhaonan Dong (*University of Leicester, United Kingdom*) 16:30

We introduce an hp -version symmetric interior penalty discontinuous Galerkin finite element method (DGFEM) for the numerical approximation of the biharmonic equation on general computational meshes consisting of polygonal/polyhedral (polytopic) elements. In particular, the stability and hp -version a priori error bound are derived based on the specific choice of the interior penalty parameters which allows for edges/faces degeneration. Furthermore, by deriving a new inverse inequality of a special class of polynomial functions (harmonic polynomials), the proposed DGFEM is proven to be stable to incorporate very general polygonal/polyhedral elements with an arbitrary number of faces for polynomial basis with degree $p = 2, 3$. The key feature of the proposed method is that it employs the elemental polynomial bases of total degree, defined in the physical coordinate system, without requiring the mapping from a given reference or canonical frame. A series of numerical experiments are presented to demonstrate the performance of the proposed DGFEM on general polygonal/polyhedral meshes.

Adaptive virtual element methods for parabolic problems using general polygonal meshes

Oliver Sutton (*University of Reading, United Kingdom*) 16:50
Andrea Cangiani (*University of Leicester, United Kingdom*)
Emmanuil Georgoulis (*University of Leicester, United Kingdom*)

This talk will present some recent advances in developing numerical schemes for solving parabolic problems using adaptive meshes consisting of general polygonal or polyhedral elements, based on the virtual element method. The adaptive algorithms we present are driven by rigorous a posteriori error estimates, developed by building on previous results for virtual element methods for elliptic problems through elliptic reconstruction techniques modified for the present setting. Numerical results will be shown to demonstrate the practical performance of these algorithms on certain benchmark problems, and the technology will be further applied to uncover new pattern forming mechanisms in a three-species cyclic competition system.

Building bridges between Galerkin methods on polytopal meshes

Simon Lemaire (*Inria, France*) 17:10

The Hybridizable Discontinuous Galerkin (HDG) method, the Virtual Element (VE) method, and the Hybrid High-Order (HHO) method are three examples of arbitrary-order Galerkin methods on general polygonal/polyhedral meshes. They are said skeletal as (and as opposed to the polytopal Discontinuous Galerkin method) cell-based degrees of freedom (DoF) can be locally eliminated in terms of boundary DoF, hence leading to global systems that are posed in terms of skeletal DoF only. It has been recently pointed out that the HHO method can be recast as

a HDG method, with distinctive numerical flux trace that ensures superconvergence on general meshes. It has also been shown that the HHO method and the nonconforming version of the VE method are equivalent (up to identical stabilization and right-hand side). We show in this presentation how to reformulate the conforming version of the VE method as a (newborn, conforming) HHO method. Doing so, we manage to unify and simplify the classical analysis of VE methods, while shedding new light on the differences between the conforming and nonconforming cases (in particular in terms of mesh requirements).

Nonconforming Trefftz virtual element method for the Helmholtz problem

Alexander Pichler (*Universität Wien, Austria*)

17:30

Ilaria Perugia (*Universität Wien, Austria*)

Lorenzo Mascotto (*Universität Wien, Austria*)

The numerical approximation of time-harmonic wave propagation problems, such as the Helmholtz problem, presents intrinsic difficulties. Due to the oscillatory nature of analytical solutions, standard (polynomial-based) Galerkin finite element methods deliver accurate approximation only at very high cost. Therefore, for these problems, finite element methods based on incorporating a priori knowledge about the differential problem to be discretized into the local approximating spaces have become increasingly popular. In literature, such methods having the feature that their test and trial functions are (locally) solutions to the targeted differential equation, are known as Trefftz methods. In this talk, we present a Trefftz virtual element method (VEM) for the approximation of solutions to the Helmholtz problem on general polygonal meshes. As typical in the VEM framework, the employed basis functions are not known in closed form, yet, by the Trefftz property, they satisfy the homogeneous Helmholtz equation. The interelement continuity constraints are imposed in a nonconforming sense. This method can be seen as an extension to the Helmholtz problem of the nonconforming harmonic VEM for the Poisson problem. Both theoretical and numerical results are discussed.

Discontinuous Galerkin approximation of flows in fractured porous media on polytopal meshes

Chiara Facciola (*Politecnico di Milano, Italy*)

17:50

Paola Francesca Antonietti (*Politecnico di Milano, Italy*)

Marco Verani (*Politecnico di Milano, Italy*)

We propose a formulation based on discontinuous Galerkin (DG) methods in their generalization to polytopic grids for the simulation of flows in fractured porous media. Our method is very flexible from the geometrical point of view, being able to handle meshes made of arbitrarily shaped elements, with edges/faces that may be in arbitrary number (potentially unlimited) and whose measure may be arbitrarily small [1], cf. also [3]. Our approach is then very well suited to tame the geometrical complexity featured by most of applications in the computational geoscience field. More precisely, we adopt a model for single-phase flows that considers the case of a single fracture, treated as a $(d-1)$ -dimensional interface between two d -dimensional subdomains, $d = 2, 3$. In the model, the flow in the porous medium (bulk) is assumed to be governed by Darcy's law and a suitable reduced version of the law is formulated on the surface modelling the fracture. The two problems are then coupled through physically consistent conditions. We focus on the numerical approximation of the coupled bulk-fracture problem, presenting and analysing, in the unified setting of [2], all the possible combinations of primal-primal, mixed-primal, primal-mixed and mixed-mixed formulations for the bulk and fracture problems, respectively. In particular, the primal discretizations are obtained using the Symmetric Interior Penalty DG method, while the mixed discretizations using the Local DG method, both in their generalization to polytopic

grids. Moreover, the coupling conditions between bulk and fracture are imposed through a suitable definition of the numerical fluxes on the fracture faces.

We perform a unified analysis of all the derived combinations of DG discretizations for the bulk-fracture problem. We prove their well-posedness and derive a priori hp-version error estimates in a suitable (mesh-dependent) energy norm.

Finally, we present numerical experiments assessing the validity of the theoretical error estimates.

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Zienkiewicz-Zhu-type error estimator on polygonal meshes

Daniel Seibel (*Saarland University, Germany*)

18:10

Steffen Weißer (*Saarland University, Germany*)

The virtual element method (VEM) and the BEM-based finite element method are effective and flexible numerical tools to solve boundary value problems on polygonal and polyhedral meshes. Typical for discretisation techniques on polytopal grids, adaptive mesh refinement strategies for the VEM and BEM-based FEM take advantage of the general structure of the meshes which include hanging nodes naturally and render post-processing to maintain the mesh admissibility unnecessary. Unfortunately, the costs of computing the error estimates and the difficulty of implementing these computations into existing code pose two serious disadvantages. The Zienkiewicz-Zhu error estimator has been originally introduced for the standard finite element method to overcome these two main problems by giving a simple and efficient alternative to existing error estimators. In this talk, we propose a new Zienkiewicz-Zhu-type error estimator for the conforming VEM for elliptic diffusion equations in 2D. We apply the basic idea of the Zienkiewicz-Zhu estimator to the VEM by defining a new quasi-interpolant which can be regarded as some sort of kernel smoothing. This quasi-interpolant together with the usual polynomial VEM projections is later used to estimate the error in such a way that the key properties of the original estimator, namely easy implementation and reduction of numerical costs, are retained. In addition, we give hints on how to extend the concept to other discretisation methods like the mentioned BEM-based FEM. Finally, we demonstrate the effectiveness of the adaptive algorithm in various numerical experiments.

YRM3 | Recent developments in damage mechanics

Date: February 18, 2019 16:30-18:30
Room: HS 21
Organiser: Philipp Junker (*Ruhr-University Bochum, Germany*)
Xiaoying Zhuang (*Leibniz University Hannover, Germany*)

Wear mechanism of hard phase containing materials

Arne Röttger (*Ruhr-Universität Bochum*) 16:30

The optimization of wear-stressed materials must be preceded by a prompt analysis of the present tribological system. Here, the individual system components are to be considered, which ultimately define the extent of material damage in their entirety. On the basis of experimental investigations, the individual micro-mechanisms of abrasion wear and surface disruption are presented. In addition to the presentation of structures of wear-resistant materials, the dominant damage mechanisms on the microscale will be presented on the basis of experimental investigations. Thereby, the individual material properties of the respectively phases (metal matrix, hard phases) will be taken into account.

On the regularization of ductile damage models

Kai Langenfeld (*TU Dortmund University, Germany*) 16:50
Jörn Mosler (*TU Dortmund University, Germany*)

Modeling softening behavior often leads to ill-posed boundary value problems. This, in turn, results in pathological mesh-dependent computations as far as the finite-element-method is concerned. A by now widely used technique to eliminate these problems is the micromorphic approach by [1, 2]. This regularization technique implicitly includes gradients of internal variables into the constitutive model. However, and in contrast to other gradient-enhanced models, the micromorphic approach preserves the local structure of the underlying local constitutive model. Within this talk, it is first shown that a naive application of this approach to ductile damage models does not work. By analyzing the respective equations, a modification of the regularization technique is elaborated - first for an isotropic ductile damage model, i.e. scalar-valued damage. Subsequently, the novel regularization is extended to tensor-valued damage models.

References

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- [2] B. J. Dimitrijevic and K. Hackl, A regularization framework for damage-plasticity models via gradient enhancement of the free energy, *International Journal for Numerical Methods in Biomedical Engineering* 27(8) (2011) 229–242

Defects detection for piezoelectric materials using isogeometric symmetric Galerkin boundary element method and level sets

B.H. Nguyen (*Leibniz-Universität Hannover, Germany*) 17:10
S.S. Nanthakumar (*Leibniz-Universität Hannover, Germany*)
X. Zhuang (*Leibniz-Universität Hannover, Germany*)

In this work, we present a flaw detection technique for piezoelectric material based on the combination of the isogeometric symmetric Galerkin boundary element method (IGA-SGBEM) and

parametric level set (PaLS)-based optimization algorithm within an iterative procedure. At each iteration, the forward problem for different void configurations is solved by IGA-SGBEM such that the objective function, which is defined by the difference between the numerical and measured boundary data (i.e. displacement and electric potential), is minimized. IGA-SGBEM appears as a natural choice, since only the boundary data is required and the change of the implicit level set function, that defines the flaws, can be easily handled in IGA without invoking re-meshing of the whole problem. Numerical examples are presented to demonstrate the robustness of the proposed method with numerical examples for both forward and inverse analysis.

An improved numerical treatment for gradient-enhanced and brittle damage modeling

Stephan Schwarz (*Ruhr-Universität Bochum, Germany*)

17:30

Dustin Roman Jantos (*Ruhr-Universität Bochum, Germany*)

Klaus Hackl (*Ruhr-Universität Bochum, Germany*)

Philipp Junker (*Ruhr-Universität Bochum, Germany*)

As is well-known, softening effects that are characteristic for damage models are accompanied by ill-posed boundary value problems arising from non-convex and non-coercive energies and resulting in mesh-dependent finite-element results. For that reason, regularization strategies that somehow take into account the non-local behavior have to be applied in order to prevent ill-posedness and to achieve mesh-independence. Hereto, most commonly gradient-enhanced formulations are considered [1,2], but also integral-type and viscous [3,4] regularization is well-known.

Gradient-enhanced damage models such as [1,2], to what group our new model [5] basically belongs, come along with a field function acting on the non-local level. Two variational equations are resulting and, however, usually the number of nodal unknowns is increased and consequently the numerical effort is increased as well.

In contrast, we present an improved algorithm for brittle damage [5] combining finite-element and meshless methods using Hamilton's principle for non-conservative continua and resulting in a quick update of the field function. Thereby, an efficient evaluation of the Laplace operator is applied as introduced in [6]. In the end, the numerical effort of the novel approach is almost comparable with an elastic problem while maintaining well-posedness and therefore mesh-independent results.

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[4] S. Schwarz, P. Junker, K. Hackl. Variational regularization of damage models based on the emulated RVE. submitted (2018)

[5] P. Junker, S. Schwarz, D.R. Jantos, K. Hackl. A fast and robust numerical treatment of a gradient-enhanced model for brittle damage. accepted (2018)

[6] D.R. Jantos, P. Junker, K. Hackl. An accurate and fast regularization approach to thermodynamic topology optimization. in review (2018)

Phase field modeling of Hertzian indentation fracture

Michael Strobl (*KIT Karlsruhe, Germany*)

17:50

Thomas Seelig (*KIT Karlsruhe, Germany*)

Phase field models of fracture have received a great deal of attention in recent years. Regularized description of cracks [1] renders Francfort and Marigo's variational model of brittle fracture easily available to compute complex crack patterns, also including e.g. mesh-independent crack nucleation from geometrically induced stress concentrations.

The present contribution focuses on the phase field simulation of fracture caused by indentation loading. Fracture initiation from the defect-free surface of a brittle solid subjected to compressive loading by a hard indenter has already been described by H. Hertz more than a century ago. Its theoretical prediction, however, is still a challenging task due to the lack of appropriate criteria for crack formation in classical fracture mechanics. The issue of indentation fracture initiation can be solved by the concept of finite fracture mechanics which comprises strength and toughness as two independent material parameters [2]. Although not directly visible, both parameters are also present in phase field formulations of fracture.

In case of indentation fracture, extensive modifications of the phase field approach are required to obtain physically reasonable results concerning crack initiation in absence of stress singularities, as observed in experiments [3], as well as the subsequent evolution of cone cracks depending on Poisson's ratio [4]. These modifications comprise constitutive assumptions to prevent damage in compressed areas but also address the role of the regularization parameter. Its suitable choice becomes one of the major questions and turns out to be a controversial issue.

Numerical results for the present non-standard problem of fracture mechanics are discussed for various indentation loading conditions and the method's capabilities are illustrated by comparison with other numerical and experimental results.

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An anisotropic brittle damage model with a damage tensor of second order using a micromorphic approach

Marek Fassin (*RWTH Aachen, Germany*)

18:10

Robert Eggersmann (*RWTH Aachen, Germany*)

Stephan Wulfinghoff (*Kiel University, Germany*)

Stefanie Reese (*RWTH Aachen, Germany*)

In the presented anisotropic damage model a damage tensor of second order is utilized. The model fulfills the damage growth criterion [1], recently published by the authors, which ensures that the stiffness of a material without healing effects decreases in any direction during a damage process (or remain at least unchanged). Noteworthy, several anisotropic damage models from the literature violate this criterion which means that artificial stiffening effects can occur. It is shown how tension compression asymmetry, which is observed for many (quasi-) brittle materials, can be incorporated into the model. Using the spectral decomposition of the strain tensor the elastic strain energy can be written in terms of a tension related part which is damaged (completely) and

a compression related part which is partially damaged or not at all. Mesh-objectivity is obtained by using a micromorphic approach in the spirit of Forest [2]. This approach represents a unifying procedure for the incorporation of gradient effects and introduces an internal length into the material model. In the micromorphic approach additional balance equations are introduced which involve additionally introduced generalized stresses. Although using a damage tensor of second order, the proposed formulation introduces only one scalar additional balance equation and therefore only one additional scalar micromorphic (nonlocal) variable, which is very efficient. In order to illustrate the effect of tension compression asymmetry, studies at integration point level are shown. By means of several structural examples the robustness of the FE formulation is demonstrated. Furthermore, mesh convergence in terms of the global force-displacement curves and the local fields are proven. In addition, the broad applicability of the model appears, which is able to represent localized damage states (fracture) as well as diffuse (distributed) damage states.

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YRM4 | Mathematical theory of deep learning

Date: February 18, 2019

16:30-18:30

Room: HS 41

Organiser: Rafael Reisenhofer (*University of Vienna, Austria*)

Philipp Petersen (*Technische Universität Berlin, Germany*)

Deep convolutional networks from sparse coding principles

Jeremias Sulam (*Johns Hopkins University, USA*)

16:30

Aviad Aberdam (*Technion, Israel Institute of Technology, Israel*)

Michael Elad (*Technion, Israel Institute of Technology, Israel*)

Sparse approximation is a well-established field, with a profound impact on signal and image processing. In this talk, we will delve into the recent multi-layer convolutional sparse model. Surprisingly, as we will carefully show, traditional deep learning architectures can be understood as implementations of pursuit algorithms under such a generative signal model. This enables us to provide global theoretical guarantees based on local sparse assumptions. We will further show how to exploit this generative model not only to analyze these networks, but also to devise ways of improving their design and performance. Concretely, I will present an alternative Holistic approach to the pursuit of such representations, giving rise to particular recurrent architectures that generalize and improve over feed-forward networks.

Optimal approximation for Wilson bases with ReLU neural networks

Dmytro Perekrestenko (*ETH Zurich, Switzerland*)

16:50

We show that finite-width deep ReLU neural networks yield rate-distortion optimal approximation (Boelcskei et al., 2017) of a wide class of functions, including polynomials, windowed sinusoidal functions, and Wilson bases. Together with the recently established universal approximation result for affine function systems (Boelcskei et al., 2017), this demonstrates that deep neural networks approximate vastly different signal structures generated by the affine group and the Weyl-Heisenberg group with approximation error decaying exponentially in the number of neurons.

Approximation spaces of deep neural networks

Felix Voigtlaender (*Catholic University of Eichstätt-Ingolstadt, Germany*)

17:10

For understanding the performance of a machine learning system, one usually considers three phenomena: generalization, optimization, and approximation (or expressiveness). In this talk, we focus only on the latter property, for the case of neural networks; that is, we systematically study the approximation capabilities of the class of neural networks, with increasing complexity (number of weights, neurons, or layers) of the networks.

In the general framework of approximation spaces, one considers a sequence $(\Omega_n)_n$ of function classes of increasing complexity; for instance, Ω_n could be the set of polynomials of degree at most n . One then classifies functions f according to how fast the best approximation error of f using functions from the class Ω_n decays as n tends to infinity. We show that if Ω_n denotes the class of neural networks of a given complexity, then all prerequisites for the general theory are satisfied, so that the corresponding approximation spaces are well-defined Banach spaces that are related by interpolation.

For neural networks using the ReLU (rectified linear unit) activation function or one of its powers, we can say more about these approximation spaces. On the one hand, many classical function spaces (Besov spaces, modulation spaces, approximation spaces of shearlets) are embedded into the neural network approximation spaces. On the other hand, at least in dimension $d=1$, if one considers network classes with a fixed depth L , then the neural network approximation spaces are embedded into certain Besov spaces. This embedding breaks down if one uses networks with an unrestricted depth. Finally, the approximation spaces have a peculiar behaviour with respect to the power of the ReLU that is used: For any two powers $n, m \geq 2$, the approximation spaces coincide, and are at least as large as the approximation spaces using just the ReLU. It is an open problem whether the approximation spaces using the ReLU function are strictly smaller than those using higher powers of the ReLU.

This is joint work with Rémi Gribonval, Morten Nielsen, and Gitta Kutyniok.

Deep learning for inverse problems. Where are we, and how far can we go?

Jonas Adler (*KTH, Sweden, Elekta, Sweden*)

17:30

Ozan Öktem (*KTH, Sweden*)

Deep learning has shown tremendous success in solving various tasks in several fields of science such as in image and natural language processing. Recently, it has also been applied to solve inverse problems and empirical evidence in image reconstruction points to drastic improvements over classical approaches.

A natural question that arises is: how good can it actually get? We try to answer this by characterizing the optimal solution given various loss functions.

In addition to this, we show that these upper bounds are empirically approximated quite well using deep neural networks.

Gabor frames and deep scattering networks in audio processing

Roswitha Bammer (*University of Vienna, Austria*)

17:50

Monika Dörfler (*University of Vienna, Austria*)

A feature extractor based on Gabor frames and Mallat's scattering transform is introduced. The resulting Gabor scattering is applied to a simple model for audio signals in order to study invariance properties and deformation stability. In particular, it is shown that different layers create invariance to certain signal features.

The decoupling technique previously used to investigate deformation stability of scattering transforms for Cartoon functions is applied to investigate to which extent the feature extractor is robust to changes in spectral shape and frequency modulation. The results are illustrated by numerical examples.

Invertible neural networks

Jens Behrmann (*University Bremen, Germany*)

18:10

Invertible deep networks provide useful theoretical guarantees and access to key quantities like densities and gradients for generative modelling. In this talk, we first review different approaches to design invertible networks. Afterwards, we discuss their ability to analyze invariants of learned representations in comparison to standard architectures. Using this analysis, we connect invariance to adversarial robustness and show how invertible networks offer a way forward.

YRM5 | Multi-physics modeling of elastomers

Date: February 18, 2019

16:30-18:30

Room: HS 07

Organiser: Vu Ngoc Khiêm (*RWTH Aachen University, Germany*)

Markus Mehnert (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

Fracture simulation by the phase-field method for polymeric materials considering rate-dependent properties

Bo Yin (*Technical University of Dresden, Germany*)

16:30

Michael Kaliske (*Technical University of Dresden, Germany*)

Since fracture plays a particularly important role in industrial application, not only experiments are adopted to investigate the complex fracture patterns, but also several numerical methodologies are intensively used to simulate crack initiation, direction, propagation as well as branching. The phase-field method has been proved to satisfy Γ -convergence of fracture, and is widely employed for structural analysis during the last decade. The phase of fracture or unfracture is indicated by a continuous scalar valued phase-field quantity. The driving force for fracture evolution can be derived from the energetic equilibrium. One of the main advantages is that the fracture evolution does not depend on any explicit criterion and does not require to trace the discontinuous displacement. Meanwhile, simulation results show good agreements with other numerical strategies or experiments.

Regarding polymeric materials, as indicated by experiments, most of them exhibit both elastic and viscous behaviour simultaneously, which yields a time dependent response. From the numerical point of view, these elastic and inelastic properties can be simulated successfully by continuum mechanical approaches. With respect to the fracture properties, rate-dependent failure needs to be investigated as well. In this work, the Bergström-Boyce model is taken into consideration for nonlinear viscoelasticity. The complexity of this model is the nonlinearity of the viscous evolution law and the mechanical response of both the equilibrium and the non-equilibrium branch. The strain energy potential supposed to evolve fracture is coming from both the equilibrium and non-equilibrium branches. The fracture mechanism is evolving from a volumetric-deviatoric energy split model, which specifies a different driving force contributing to the fracture when the solid is undergoing a tension or compression state. This work is formulated and implemented in the context of the Finite Element (FE) framework. For verification and evaluation, numerical examples are performed and discussed. Last but not least, conclusions and future perspectives close this presentation.

Coupled thermomechanical model for strain induced crystallization in polymers

Serhat Aygün (*TU Dortmund University, Germany*)

16:50

Sandra Klinge (*TU Dortmund University, Germany*)

Crystallization in certain polymers, like natural rubber, is characterized by the specific geometrical arrangement of atoms in macromolecules caused by high strains. Starting from crystallization nuclei, polymer chains leave their natural entangled structure, stretch out, fold back and stack. Eventually, they build regions with a regular structure, also called lamellae. The process must be taken into consideration when planning manufacturing processes since it significantly influences mechanical and thermal properties of the final product. The present contribution deals with the thermomechanical model for crystallization of unfilled polymers, which involves

displacements and temperature as global degrees of freedom, and the degree of network regularity as an internal variable. The mechanical part of the model uses the dissipation potential developed in our previous work [1]. Such an approach has two special features: Firstly, the thermodynamically consistent framework is developed to simulate the reduction of the network regularity during the unloading phase. Secondly, the microstructure evolution under the cyclic tensile load is visualized. The thermal part of the model is based on the solution of the heat conduction equation. Moreover, the Fourier's law in reference configuration provides the relationship between the temperature distribution and heat flux. The resulting, coupled thermomechanical problem is solved in a monolithic way. Finally, selected numerical examples are compared with experimental data of natural rubber without fillers.

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Thermo-micromechanics of strain-induced crystallization based on the analytical network-averaging concept

Vu Ngoc Khiêm (*RWTH Aachen University, Germany*)

17:10

Mikhail Itskov (*RWTH Aachen University, Germany*)

Crystallization is the transformation of amorphous polymer chains to perfect order molecular structures (crystallites). The exceptionally high stereo-regularity of natural rubber allows it to crystallize when undergoing deformation. Strain-induced crystallites are supposed to play an important role in the elastomer reinforcement and enhance the resistance to crack growth in natural rubbers. In this contribution, we present a thermo-micromechanical theory of strain-induced crystallization in natural rubbers based on the analytical network-averaging concept (Khiêm and Itskov 2018). Accordingly, the phase transition is accompanied by heat production (absorption) and induces an evolution of the heat source. In contrast to previous works on thermo-mechanics of rubber-like materials, the internal energy and the entropy of the representative chain are formulated in our model explicitly in terms of state variables. The crystallization kinetics delivers microscopic boundary conditions for the representative chain on the one hand, and provides a formulation for the crystallinity on the other hand. Model predictions are compared with comprehensive experimental results and shed new light on strain-induced crystallization of natural rubbers.

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Modeling electro-elastic coupling phenomena of electroactive polymers in the context of structural mechanics

Elisabeth Hansy-Staudigl (*Vienna University of Technology, Austria*)

17:30

Michael Krommer (*Vienna University of Technology, Austria*)

Yury Vetyukov (*Vienna University of Technology, Austria*)

Alexander Humer (*Johannes Kepler University Linz, Austria*)

Bringing into focus the design aspect of thin film electro-active polymer actuators justifies the deployment of a structural mechanics framework. We propose a physically consistent constitutive model for such actuators, which is valid for plates and shells as material surfaces within a complete direct formulation. To this end, we use the principle of virtual work to deduce the general form of the constitutive law from an augmented Helmholtz energy, as a function of the structural Green-Lagrange type strain measures and of the electric field, without the need of *a-priori* assumptions concerning the state of strain and stress.

Mechanical deformations of thin film devices - e.g. made of polyurethane - under the action of an external electric field, are caused by two different sources. On the one hand, the applied electric field causes a dielectric polarization of the polymer matrix, yielding to corresponding attractive electrostatic forces between the electroded surfaces resulting into a squeezing of the film. On the other hand, crystalline graft units with a certain natural, but arbitrarily directed polarization, embedded in between the polymer chains, have to align to the direction of the applied electric field such that a rotation of the whole crystal unit takes place. This rotation results in an additional macroscopic thickness squeeze - known as the electrostrictive effect.

We treat both electromechanical coupling phenomena separately, where it turns out, that the electrostatic forces can be accounted for by an electrical contribution to the augmented free energy, whereas, the electrostrictive effect is taken into account in the elastic part of the augmented free energy by virtue of a hybrid multiplicative and additive decomposition of the plate/shell deformation measures.

Benefiting from the structural mechanics formulation, we gain a lower, two-dimensional, formulation, which provides a clear physical insight into the nature of the deformation process initiated by the external electric field. E.g. for the linearised problem, a comparison to the literature on thermoelastic plates and shells uncovers the action of the electric field as a combined source of self-stresses and eigenstrains. In order to solve particular problems, the constitutive relation of the geometrically and physically nonlinear formulation is implemented into our in-house finite element code. The computed results, which were tested against results from the literature as well as against test problems of our previous work (where numerical integration of the three dimensional plate/shell augmented free energy through the thickness was employed), show a very good agreement.

Electro-mechanical characterization of VHB 4905

Markus Mehnert (*University of Erlangen-Nuremberg, Germany*)

17:50

Mokarram Hossain (*Swansea University, UK*)

Paul Steinmann (*University of Erlangen-Nuremberg, Germany*)

During the past years an increased interest in so called smart materials due to new demands in the development of state-of-the-art technology could be observed. One promising representative of these smart materials is the group of electro-active polymers (EAPs). These polymeric materials react with large deformations and a change in their material properties to the excitation by an electric field. This renders them interesting candidates for the use as soft generators or other commercial applications such as adaptive stiffness actuators, adaptive lenses in optics or even artificial muscles. Due to the expensive and time consuming nature of real-life experimental work there is a high demand for the simulation of these innovative materials using numerical solution approaches such as the finite-element method. In this contribution we present a number of experimental works conducted on VHB 4905, a commercially available dielectric polymer from 3M. Furthermore we present an electro-viscoelastic modelling approach with field dependent material parameters based on the work of Hossain et al. that can be used for the simulation of electro-active polymers. We select an eight-chain model for the ground state elasticity whereas the viscous material behavior is represented by a Neo-Hookean type model using the linear evolution equation proposed by Lubliner. The derived material model is implemented into an in house finite-element code using the FE library deal.II. The necessary material parameters are identified using the conducted experiments. Finally we present a comparison between the experiments and the simulations.

Reduced-order modelling and computational homogenisation of magnetorheological elastomers

Benjamin Brands (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*) 18:10
Denis Davydov (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)
Julia Mergheim (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)
Paul Steinmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

The mechanical response of magnetorheological composites is highly affected by an applied magnetic field. Since a generally valid constitutive law does not exist for such heterogeneous materials, multiscale techniques like computational homogenisation are commonly used to approximate effective macroscopic properties. In our approach the macroscopic quantities at a material point of a magnetorheological elastomer are derived from the response of the underlying micro-structure, where the constitutive law is known, using first-order homogenisation.

The computational cost of this nested solution scheme known as the FE^2 method prohibits the simulation of complex macroscopic problems. To mitigate the computational bottleneck the FE models on the microscale are replaced by reduced-order models (ROMs). In projection-based ROM the governing equations are projected onto the reduced basis, which is an approximation of the solution manifold of the parametrised partial differential equations (pPDE). The reduced basis is commonly constructed using previously computed solutions of the pPDE, e.g. by applying proper orthogonal decomposition or the reduced basis method.

We will present our approach for the construction and computation of the reduced-order models on the microscale. Through various numerical examples the accuracy and time savings of the reduced models will be discussed.

DFG Priority Programs

DFG-PP 1748 | Reliable simulation techniques in solid mechanics. Development of non-standard discretization methods, mechanical and mathematical analysis

Date: February 19, 2019 14:00-16:00
Room: HS 32
Organiser: Jörg Schröder (*University of Duisburg-Essen, Germany*)
Thomas Wick (*Leibniz University Hannover, Germany*)

A new C0-continuous finite element formulation for gradient elasticity

Johannes Riesselmann (*Ruhr-Universität Bochum, Germany*) 14:00
Jonas Ketteler (*Universität Münster, Germany*)
Mira Schedensack (*Universität Münster, Germany*)
Daniel Balzani (*Ruhr-Universität Bochum, Germany*)

Gradient elasticity formulations enable the modeling of size-effects. These can be observed e.g., in materials in which microstructural length parameters have an influence on the constitutive behavior. The idea is to incorporate not only first order deformation gradients into the elastic free energy function but also second-order gradients. Furthermore, due to this gradient enrichment, geometry-induced nonphysical singularities which can occur in classical formulations are prevented. However, in a pure displacement formulation such nonlocal models require C1-continuous approximations. Alternative mixed formulations, which include deformations as well as other fields associated with the gradients may however be expensive. In this contribution a novel approach is proposed, in which deformation gradients are taken as the only independent variable by incorporating the rotation-free condition of gradient fields as constraint. This way a C0-continuous approximation is possible and a cost reduction compared to other mixed formulations can be achieved. Comparative numerical studies reveal an appropriate convergence behavior also in the large strain framework. In conclusion, a new finite element technology is proposed whose transfer to other problems (e.g. gradient damage) appears promising.

A posteriori error control for the finite cell method

Andreas Schröder (*Universität Salzburg, Austria*) 14:20
Davide D'Angella (*Technische Universität München, Germany*)
Paolo Di Stolfo (*Universität Salzburg, Austria*)
Alexander Düster (*Technische Universität Hamburg, Germany*)
Simeon Hubrich (*Technische Universität Hamburg, Germany*)
Stefan Kollmannsberger (*Technische Universität München, Germany*)
Ernst Rank (*Technische Universität München, Germany*)

The finite cell method is a combination of a fictitious domain method with a finite element method. Its basic idea is to replace the possibly complicated physical domain by an embedding domain of a geometrically simple shape, for instance, a (paraxial) quadrilateral in 2D or a (paraxial) hexahedron in 3D, which can easily be meshed. The variational formulation of the problem and its finite element discretization is defined on the embedding domain. The geometry of the physical domain is incorporated via an indicator function which necessitates the implementation of an appropriate quadrature scheme. This can be done by using an additional quadrature mesh, which approximates the physical domain and, thus, implies a certain quadrature error. Hence, mainly two computational error sources occur in the finite cell method: the

discretization error and the quadrature error. In this talk, we present some concepts of the finite cell method and discuss a posteriori error control for this method. The focus is on the application of the dual weighted residual approach (DWR) enabling the control of the error with respect to a user-defined quantity of interest. The aim is to estimate both the discretization error and the quadrature error. The application of the DWR approach provides an adaptive strategy in which the error contributions resulting from discretization and quadrature are balanced. The strategy consists in either refining the finite cell mesh or its associated quadrature mesh. In several numerical experiments the performance of the error control and the adaptive scheme is demonstrated for linear and nonlinear problems in 2D.

A posteriori estimator for the adaptive solution of a quasi-static fracture phase field model

Mirjam Walloth (*Technische Universität Darmstadt, Germany*)

14:40

Katrin Mang (*Leibniz Universität Hannover, Germany*)

Thomas Wick (*Leibniz Universität Hannover, Germany*)

Winnifried Wollner (*Technische Universität Darmstadt, Germany*)

In the numerical simulation of fracture propagation phase-field models are widely used. The unknowns of the system are the deformation u of the elastic body and the phase-field variable ϕ which describes a diffusive transition zone between the broken ($\phi=0$) and the unbroken material ($\phi=1$). This zone has a half bandwidth ϵ , which is a model regularization parameter. The phase-field variable is constrained by the irreversibility condition, i.e. $\phi^{n+1} \leq \phi^n$ where n denotes the time step. Thus, we get a quasi-static coupled system of an equation and an inequality. For the discretization we use finite elements. The arising discrete system can be solved either by a monolithic approach [1] or by means of an alternating minimization method [2] where the equation and the inequality are solved alternately.

As there is no a priori information about the local regularity of the resulting non-linear and non-smooth system a posteriori estimators are an important tool to detect regions where the solution is less regular or even singular.

We are especially interested in a good approximation of the fracture growth.

Therefore we develop a residual-type a posteriori estimator for the variational inequality of the phase-field variable.

Due to the irreversibility constraint standard residual a posteriori estimators are inappropriate. They would cause an overestimation where the constraints are active which is for example in the unbroken area. Thus, in order to derive a reliable and efficient residual-type a posteriori estimator we follow a new approach [3] for variational inequalities and measure the error in the phase-field variable and the corresponding constraining force. Further, the estimator should be robust as the variational inequality is singularly perturbed. Therefore we use an energy norm to measure the error in ϕ and the corresponding dual norm to measure the error in the constraining forces. The estimator we will present constitutes an upper bound and local lower bounds for this error measure. Numerical results will demonstrate the efficiency and robustness with respect to the model regularization parameter ϵ .

References:

- [1] T. Wick, An error-oriented Newton/inexact augmented Lagrangian approach for fully monolithic phase-field fracture propagation., *SIAM J. Sci. Comput.* 39 (4), pp. B589–B617, 2017.
- [2] S. Burke, C. Ortner, and E. Süli, An adaptive finite element approximation of a variational model of brittle fracture., *SIAM J. Numer. Anal.* 48 (3), pp. 980–1012, 2010.
- [3] R. Krause, A. Veese, M. Walloth, An efficient and reliable residual-type a posteriori error estimator for the Signorini problem. *Numer. Math.* 130, pp. 151–197, 2015.

Adaptive isogeometric discretizations for diffuse modelling of discontinuities

Markus Kästner (*Technische Universität Dresden, Germany*)

15:00

Paul Hennig (*Technische Universität Dresden, Germany*)

Roland Maier (*Universität Augsburg, Germany*)

Daniel Peterseim (*Universität Augsburg, Germany*)

In the numerical analysis of heterogeneous materials, weak and strong discontinuities arise in the field variables due to rapidly changing mechanical properties at material interfaces or due to propagation of cracks if a specific failure load is exceeded.

Details about the local topology of heterogeneous microstructures are typically taken from imaging methods or are given in terms of random distributions. To avoid costly meshing processes, embedded domain methods, that represent the physical domain implicitly in a regular background mesh, can be used. While good convergence rates are achieved for homogeneous materials, stress oscillations occur in the heterogeneous case because weak discontinuities are modeled in terms of a continuous basis.

For that reason, we propose a regularization of the sharp material interfaces over a newly introduced length scale. To define the material properties in the transition region, homogenization assumptions are used that fulfill the balance of linear momentum at the interface and kinematic compatibility. Adaptive h-refinement based on hierarchical B-splines is applied to provide a local refinement strategy, where element size and regularization length are reduced simultaneously. The convergence behavior of this approach is tested in different benchmark problems.

To account for local damage and failure, the modeling of the heterogeneous material structure is extended by a phase-field model for bulk and interface cracks. In this way, cumbersome topological updates of the analysis mesh to track the crack path, are avoided. Crack initiation and propagation are accounted for by solving an additional scalar field problem that is coupled to the mechanical one.

To simulate interface failure between two materials, we combine the phase-field model with a local reduction of the critical fracture energy in the area of the regularized material interface. The method considers possible interactions between the regularization of the interface and the phase-field and ensures crack propagation with the experimentally observed fracture toughness of the interface.

Eventually, we demonstrate the proposed modeling approach in numerical examples for crack propagation in heterogeneous materials using the embedded domain method.

Quasi-collocation methods for isogeometric and stochastic finite-element-analysis

Hermann G. Matthies (*TU Braunschweig, Germany*)

15:20

Frederik Fahrenndorf (*TU Braunschweig, Germany*)

Laura de Lorenzis (*TU Braunschweig, Germany*)

Bojana Rosic (*TU Braunschweig, Germany*)

Sharana K. Shivanand (*TU Braunschweig, Germany*)

In any deterministic and/or stochastic finite-element (FE) analysis, usually integrals have to be computed for the Galerkin- and / or pseudo-spectral projection, typically by some numerical quadrature rule. The evaluation of the integrand at the quadrature points can be a major computational expense, so that there is a desire to reduce the number of integration or quadrature point as much as possible. Collocation methods can be viewed as such an attempt of having the minimum number necessary to ensure full rank of the corresponding matrices and their positive definiteness and thus allow a unique numerical solution. Unfortunately, classical collocation

methods may be prone to instabilities. Here we study quasi collocation, which is the possibility of viewing the collocation method as a reduced integration scheme. The idea is to define stable methods with as few quadrature points as possible.

Isogeometric analysis (IGA) is based on the idea of discretising both the design and the analysis model for a deterministic simulation by higher-order basis functions stemming from computer-aided design, such as non-uniform rational B-Splines (NURBS). For an efficient implementation of a Galerkin-FE approach in the IGA framework, standard Gaussian quadrature rules are not well-suited, since they do not take advantage of the higher continuity of the shape functions. As a possible remedy, a reduced quadrature technique originating from the concept of variational collocation has been studied. The determination of the quadrature points has been realised on the basis of superconvergence theory and leads (in case of odd degrees) to two quadrature points per parametric direction independently of the degree of the discretisation.

In a stochastic FE-Method (SFEM) integrals over very high-dimensional domains have to be computed either for the Galerkin-projection or for the inner products of a pseudo-spectral projection, and this is often approached classically via (Quasi) Monte Carlo integration, or more recently via sparse-grid Smolyak quadrature. Whereas (Quasi) Monte Carlo methods require and use very little of possible smoothness and regularity properties of the integrand, sparse-grid Smolyak methods (which unfortunately have partly negative quadrature weights) are very sensitive in this regard. Here we start with (Quasi) Monte Carlo methods, but add regularity assumptions in a Bayesian fashion. The idea is to see the integral as an unknown / uncertain quantity which is to be estimated via samples of the integrand. Prior assumptions can be introduced in a Bayesian setting through the specification of an appropriate prior. After computing a new sample of the integrand at a new quadrature point, the estimate of the integral is evaluated via Bayesian updating. This puts this approach in the realm of probabilistic numerics.

The alternating direction method of multipliers with variable step sizes and its application to the simulation of BV-damage evolution

Marijo Milicevic (*Universität Freiburg, Germany*)

15:40

Sören Bartels (*Universität Freiburg, Germany*)

Marita Thomas (*Weierstraß-Institut, Germany*)

The alternating direction method of multipliers (ADMM) is a flexible numerical method to solve a large class of convex minimization problems. Its most significant properties are the unconditional convergence with respect to the involved step size and the direct applicability. However, the performance critically depends on the choice of the step size. We propose an automated step size adjustment that relies on the monotonicity of the residual to accelerate the ADMM. Numerical experiments show a remarkable improvement over the standard ADMM with fixed step sizes. The ADMM with variable step sizes is then applied to a model for rate-independent, total variation regularized damage processes. The total variation regularization of the damage variable leads to sharp transitions of damaged to undamaged areas in the material. The results are compared with an H^1 -regularization of the damage and the simulations reveal that, indeed, for the total variation regularization sharp transitions can be observed whereas for the H^1 -regularization the interface is smeared out.

DFG-PP 1798 | Compressed sensing in information processing (CoSIP)

Date: February 19, 2019 14:00-16:00
Room: HS 02
Organiser: Gitta Kutyniok (*Technische Universität Berlin, Germany*)
Rudolf Mathar (*RWTH Aachen University, Germany*)

Robust one-bit compressed sensing with non-Gaussian measurements

Sjoerd Dirksen (*RWTH Aachen, Germany*) 14:00
Shahar Mendelson (*The Australian National University, Canberra, Australia*)

In the traditional compressed sensing literature, it is implicitly assumed that one has direct access to noisy analog linear measurements of an (unknown) signal. In reality, these analog measurements need to be quantized to a finite number of bits before they can be transmitted, stored, and processed. In the emerging theory of quantized compressed sensing it is studied how to jointly design a quantizer, measurement procedure, and reconstruction algorithm in order to accurately recover low-complexity signals.

In the popular one-bit compressed sensing model, each linear analog measurement is quantized to a single bit in a memoryless fashion. This quantization operation can be implemented with energy-efficient hardware. There is by now a rich theory available for one-bit compressed sensing with standard Gaussian measurements. Outside of this purely Gaussian setting, very little is known about one-bit compressed sensing. In fact, recovery can in general easily fail for non-Gaussian measurement matrices, even if they are known to perform optimally in ‘unquantized’ compressed sensing.

In my talk, I will show that this picture completely changes if one uses dithering, i.e., deliberately adds noise to the measurements before quantizing them. By using well-designed dithering, it becomes possible to accurately reconstruct low-complexity signals from a small number of one-bit quantized measurements, even if the measurement vectors are drawn from a heavy-tailed distribution. The reconstruction results that I will present are very robust to noise on the analog measurements as well as to adversarial bit corruptions occurring in the quantization process. If the measurement matrix is subgaussian or subgaussian circulant, then accurate recovery can be achieved via a convex program.

Based on joint work with Shahar Mendelson (ANU Canberra)

Low rank recovery from phaseless inner products with matrix groups

David Gross (*University of Cologne, Germany*) 14:40
Ingo Roth (*Free University Berlin, Germany*)
Richard Kueng (*California Institute of Technology, USA*)
Shelby Kimmel (*Middlebury College, USA*)
Yi-Kai Liu (*National Institute of Standards and Technology, USA*)
Jens Eisert (*Free University Berlin, Germany*)
Martin Kliesch (*University of Duesseldorf, Germany*)

We consider the problem of recovering a unitary map from phaseless inner products with randomly chosen elements of a matrix group. The problem occurs in quantum information. There, such phaseless inner products can be estimated in a particularly robust way using a protocol known as "randomized benchmarking". Combining methods from compressed sensing and representation theory, we provide a number of near-optimal recovery guarantees for this problem, including its generalization from unitary to "completely positive" maps. Main reference: arxiv.org:1803.00572.

Learning the invisible

Tatiana A. Bubba (*University of Helsinki, Finland*) 15:00
Gitta Kutyniok (*Technische Universität Berlin, Germany*)
Matti Lassas (*University of Helsinki, Finland*)
Maximilian März (*Technische Universität Berlin, Germany*)
Wojciech Samek (*Fraunhofer Heinrich Hertz Institute, Germany*)
Samuli Siltanen (*University of Helsinki, Finland*)
Vignesh Srinivasan (*Fraunhofer Heinrich Hertz Institute, Germany*)

A Hybrid Deep Learning-Shearlet Framework for Limited Angle Computed Tomography
The high complexity of various inverse problems poses a significant challenge to model-based reconstruction schemes, which in such situations often reach their limits. At the same time, we witness an exceptional success of data-based methodologies such as deep learning. However, in the context of inverse problems, deep neural networks mostly act as black box routines, used for instance for a somewhat unspecified removal of artifacts in classical image reconstructions. In this talk, we will focus on the severely ill-posed inverse problem of limited angle computed tomography, in which entire boundary sections are not captured in the measurements. We will present a hybrid reconstruction framework that fuses model-based sparse regularization with data-driven deep learning. Our method is reliable in the sense that we only learn the part that can provably not be handled by model-based methods, while applying the theoretically controllable sparse regularization technique to the remaining parts. Such a decomposition into visible and invisible segments is achieved by means of the shearlet transform that allows to resolve wavefront sets in the phase space. This split furthermore enables us to assign the clear task of inferring unknown shearlet coefficients to the neural network and thereby offering an interpretation of its performance in the context of limited angle computed tomography.

Analysis of the generalization error: empirical risk minimization over deep artificial neural networks overcomes the curse of dimensionality in the numerical approximation of black-scholes partial differential equations

Julius Berner (*University of Vienna, Austria*) 15:20
Philipp Grohs (*University of Vienna, Austria*)
Arnulf Jentzen (*ETH Zürich, Switzerland*)

The development of new classification and regression algorithms based on empirical risk minimization (ERM) over deep neural network hypothesis classes, coined Deep Learning, revolutionized the area of artificial intelligence, machine learning, and data analysis. More recently, these methods have been applied to the numerical solution of high dimensional partial differential equations (PDEs) with great success. In particular, recent simulations indicate that deep learning based algorithms are capable of overcoming the curse of dimensionality for the numerical solution of linear Kolmogorov PDEs. Kolmogorov PDEs have been widely used in models from engineering, finance, and the natural sciences. In particular Kolmogorov PDEs are highly employed in models for the approximative pricing of financial derivatives. Nearly all approximation methods for Kolmogorov PDEs in the literature suffer under the curse of dimensionality. By contrast, in recent work by some of the authors it was shown that deep ReLU neural networks are capable of approximating solutions of Kolmogorov PDEs without incurring the curse of dimensionality. The present paper considerably strengthens these results by providing an analysis of the generalization error. In particular we show that for Kolmogorov PDEs with affine drift and diffusion coefficients and a given accuracy $\epsilon > 0$, ERM over deep neural network hypothesis classes of size scaling polynomially in the dimension d and ϵ^{-1} and with a number of training samples

scaling polynomially in the dimension d and ϵ^{-1} approximates the solution of the Kolmogorov PDE to within accuracy ϵ with high probability. We conclude that ERM over deep neural network hypothesis classes breaks the curse of dimensionality for the numerical solution of linear Kolmogorov PDEs with affine drift and diffusion coefficients. To the best of our knowledge this is the first rigorous mathematical result that proves the efficiency of deep learning methods for high dimensional problems.

A gridless CS approach for channel estimation in hybrid massive MIMO systems

Khaled Ardah (*Ilmenau University of Technology, Germany*)

15:40

André L. F. de Almeida (*Federal University of Ceará, Brazil*)

Martin Haardt (*Ilmenau University of Technology, Germany*)

Channel state information estimation in hybrid analog-digital millimeter-wave massive MIMO systems is a challenging problem due to the high channel dimension and reduced number of radio-frequency chains. However, exploiting the channel sparsity, several methods have been proposed leveraging the compressed sensing (CS) tools. Most of the prior works consider an approximate CS formulation by assuming that the channel parameters lie perfectly on a finite grid neglecting the grid mismatch effect. To resolve this issue, we propose a gridless CS approach that exploits of the antenna array geometry. The proposed algorithm is based on an alternating optimization technique and is guaranteed to converge to a local minimum. Simulation results are provided to evaluate the effectiveness of the proposed algorithm.

DFG-PP 1886 | Polymorphic uncertainty modelling for the numerical design of structures

Date: February 19, 2019

14:00-16:00

Room: HS 42

Organiser: Michael Kaliske (*Technische Universität Dresden, Germany*)

Application of recurrent neural networks in structural analysis of concrete structures considering polymorphic uncertainty

Ferenc Leichsenring (*Technische Universität Dresden, Germany*)

14:00

Alexander Fuchs (*Technische Universität Dresden, Germany*)

Wolfgang Graf (*Technische Universität Dresden, Germany*)

Michael Kaliske (*Technische Universität Dresden, Germany*)

The realistic modelling of structures is fundamental for their numerical simulations and is mainly characterized by the mechanical model and the consideration of the available data at hand by an adequate uncertainty model.

The key idea in this contribution is the consideration of polymorphic uncertainty at the numerical structural analysis and the mechanical modelling for reinforced concrete structures, which are characterized by a combination of heterogeneous concrete and different types of reinforcement (e.g. steel bars or woven carbon fibres). Typically, the reinforcement is denoted by another length scale, compared to the overall structure size. The formulation and development of a computational homogenization approach, considering the different homogeneous and heterogeneous characteristics of a macroscopic structure, is essential for a precise numerical computation. In recent years, focal point of research was on structural analysis considering uncertain material or geometry parameters. Probabilistic approaches are dominating the uncertainty consideration currently, although they are connected with certain disadvantages and limits. In this contribution, a generalized uncertainty model is utilized in order to take variability, impression as well as inaccuracy, vagueness and incompleteness into account. That allows a separated evaluation of the influence for each uncertainty source on the results. Therefore, polymorphic uncertainty models are applied and developed by combining and extending aleatoric and epistemic uncertainty, resulting e.g. in the formulation of the uncertainty model “fuzzy probability based randomness”. The information of the different length scales is considered to be uncertain, e.g. the geometry or the material properties of a representative volume element (RVE) at the meso scale. Subsequently, the uncertainty of a macro structure is derived from uncertain results on the meso structure. In the contribution a parametrized RVE for concrete structures, including cement phase as well as aggregates, is presented. Various material parameters are considered as uncertain, which results in uncertain effective quantities. Assuming, that an uncertain quantity is substitutable by a combination of a representative measure and multiple uncertainty characterizing measures, an approximation of both type of quantities by a recurrent neural network is carried out. The surrogate models are utilized as constitutive description in a numerical structural analysis on macro level, providing uncertain structural responses.

Polymorphic uncertainty propagation with application to failure analysis of adhesive bonds in rotor blades

Martin Drieschner (*Technical University of Berlin, Germany*)

14:20

Martin Eigel (*Weierstrass Institute for Applied Analysis and Stochastics (WIAS Berlin)*)

Robert Gruhlke (*Weierstrass Institute for Applied Analysis and Stochastics (WIAS Berlin)*)

Dietmar Hömberg (*Weierstrass Institute for Applied Analysis and Stochastics (WIAS Berlin)*)

Yuriy Petryna (*Technical University of Berlin, Germany*)

This contribution was developed within the research project MuSca-BlaDes: Multi-scale failure analysis with polymorphic uncertainties for optimal design of rotor blades, which is part of the DFG Priority Program (SPP 1886): Polymorphic uncertainty modelling for the numerical design of structures started in 2016.

One of the typical failure mechanisms of rotor blades in operation is the cracking of adhesive bonds in the load-bearing structure, on which we focus in our project. Based on manufacturing processes, the failure is accompanied by several polymorphic uncertainties including air voids characterized by amount, shape, size and distribution [1].

We discuss recent results obtained in the modeling and approximation of the underlying polymorphic linear elastic partial differential equation [2]. In particular we compare quantities of interests of the polymorphic solution based on the micro modeled adhesive bond and compare them to polymorphic meso scale solutions obtained by using upscaled random material. The latter is constructed within a Bayesian framework using an appropriate prior model of the underlying meso scale material in the forward model. Real experiments are used to validate the uncertainty model.

[1] D. Kovacevic, Y. Petryna, M. Petronijevic, Assessment of the impact of air voids on adhesive joints in rotor blades by use of NDT and FEA. EWSHM, 2016.

[2] M. Drieschner, R. Gruhlke, Polymorphic uncertainty propagation with application to perforated acrylic glass. In preparation, 2018

Polymorphic uncertainty quantification in acoustic systems

Thomas Kohlsche (*Technische Universität Hamburg, Germany*)

14:40

Stephan Lippert (*Technische Universität Hamburg, Germany*)

Otto von Estorff (*Technische Universität Hamburg, Germany*)

The numerical simulation of acoustic problems is, for itself, a quite difficult task, since the underlying systems are usually highly complex with a broad frequency range and high sensitivity. Due to this complexity and the corresponding computational burden, tasks like optimization and uncertainty quantification (UQ) are seldom performed in acoustics. Especially when dealing with polymorphic uncertainties, where combined techniques of UQ have to be applied, a direct use of the model is not applicable.

To tackle this problem, the computational costs have to be lowered significantly. In most UQ application, standard model order reduction techniques or surrogate models are used. For acoustics, standard approaches often get in particular trouble due to resonance and interference phenomena which cause highly non-linear, peak-like local responses. Therefore, it is mandatory for such problems to find an approach for model reduction to make UQ accessible at all.

This contribution deals with possibilities to reduce acoustic systems such that both the relevant global and local characteristics are retained. The techniques will be applied on an acoustic test system to demonstrate their capabilities.

Polymorphic Uncertainty Quantification via Hierarchical Low Rank Tensors

Lars Grasedyck (*RWTH Aachen, Germany*)

15:00

Dieter Moser (*RWTH Aachen, Germany*)

We consider a PDE model problem with uncertain parameters of varying type ranging from classical stochastic unknowns to parameters defined by bounds or in fuzzy terms. For these inputs we first determine the mapping from all parameters to quantities of interest in high dimensional but hierarchical low rank form. Subsequently we use the compressed hierarchical representation in order to describe the possible output quantities.

Some theoretical aspects of the spectral Fuzzy FEM

Dmytro Pivovarov (*Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg, Germany*)

15:20

Kai Willner (*Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg, Germany*)

Paul Steinmann (*Chair of Applied Mechanics, Friedrich-Alexander University Erlangen-Nürnberg, Germany*)

In this work we review some modifications for the fuzzy FEM involving spectral representation of the uncertainties. We address some theoretical aspects of fuzzy FEM, that haven't been widely discussed before, namely the inner product of fuzzy variables. We address also another important problem, which becomes often the target of criticism of fuzzy approach. The membership function of the fuzzy input has often some degree of arbitrariness: it is known only approximately or it is constructed based on some assumptions. Here we propose a fuzzy output representation, which requires only the modal value and support of the fuzzy input parameters and is completely independent of the input membership function's shape.

Uncertainty Quantification in Fluid Mechanics and Fluid-Structure Interaction Using Cheap Approximators

Jonas Nitzler (*Technical University of Munich, Germany*)

15:40

Jonas Biehler (*Technical University of Munich, Germany*)

Phaedon-Stelios Koutsourelakis (*Technical University of Munich, Germany*)

Wolfgang A. Wall (*Technical University of Munich, Germany*)

This contribution addresses Uncertainty Quantification (UQ) for complex multi-physics problems using novel Bayesian multi-fidelity approaches which exploit low-fidelity models to reduce the overall computation costs [1, 3-5].

The use of classical sampling based techniques would require a vast amount of simulation runs of the high-fidelity model for an accurate assessment of the response statistics and probability distributions of simulation outputs. As this is mostly not feasible due to limited resources the novel frameworks aim to overcome the computational drawbacks of classical UQ methods. In contrast to multi-level Monte Carlo methods (MLMC) [2], the Bayesian schemes are capable of capturing even strong non-linearities and noisy correlations leading to so far unreached accuracies as well as speed-ups. The presented approaches are furthermore very robust and allow for a wide variety of low-fidelity models.

Here, we will investigate fluid simulations and fluid-structure interactions with uncertain model inputs to demonstrate the method's ability to handle complex systems. Computationally cheap

approximators can be motivated by the use of simplified physics, coarser discretizations or relaxed coupling conditions. In this work we will focus on the simultaneous use of several low fidelity models and their impact on the overall result accuracy and efficiency gain.

References

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DFG-PP 1897.01 | Calm, smooth and smart - novel approaches for influencing vibrations by means of deliberately introduced dissipation

Date: February 19, 2019

14:00-16:00

Room: HS 41

Organiser: Peter Eberhard (*University of Stuttgart, Germany*)

A numerical model for analysis of design parameters for particle dampers

Niklas Meyer (*Hamburg University of Technology, Germany*)

14:00

Robert Seifried (*Hamburg University of Technology, Germany*)

Lightweight designs are becoming increasingly important these days to reduce energy consumption and natural resources. However, a smaller weight typically causes a decrease in stiffness and non-negligible vibration amplitudes over a wide frequency range. One passive technique to reduce these vibrations is the use of particle dampers. Thereby containers attached to a vibrating structure or holes embedded in the vibrating structure are filled with granular material. Due to the structural vibrations, momentum is transferred to the granular material which interacts with each other. As a result, energy is dissipated by impacts and frictional phenomena between the particles.

Particle dampers show several advantages when compared to other existing passive damping techniques. They may be insensitive to temperature and environmental conditions, do not necessarily add significant mass and do not degrade in time. In literature it has been shown that they are at least as effective as other damping techniques, and the effectiveness is not restricted to a single frequency but exists over a broader frequency range.

The efficiency of particle dampers has been demonstrated experimentally in a few different engineering applications. However, so far the damper design has been based on very specific systems. This might be due to the fact, that the processes in the particle dampers are highly nonlinear and depend on a variety of different influence parameters, like the excitation frequency, and vibration amplitude.

In this presentation, the development of a coupled discrete element-reduced finite element model for analysis of the damping behavior for multiple eigenfrequencies is presented. Thereby the frequency response and the damping ratio are extracted from such a simulation model.

An experimental setup to validate the numerical model is used, consisting of a beam supported by soft cables to represent a free-free boundary condition. On the structure a box, filled with particles, is mounted at different locations. The beam is excited by a shaker and a laser scanning vibrometer is used to determine the frequency response and thus the modal parameters.

With the numerical model and the experimental setup the influence of design parameters on the particle damper efficiency for a wide frequency range are performed. It is analyzed how the different modal parameters are affected by the position of the particle damper, its filling ratio and the granular material. These results should be further used for the development of macro-models, which can be used in simulation of larger structures with several attached particle dampers.

Investigating the effect of complex particle shapes in liquid filled particle dampers using coupled DEM-SPH methods

Peter Eberhard (*University of Stuttgart, Germany*)

14:20

Chandramouli Gnanasambandham (*University of Stuttgart, Germany*)

The process of energy dissipation in particle dampers (PD) occurs mainly due to relative motion between solid particles within the damper container. The degree of relative motion between

solid particles is especially sensitive to vibration amplitude changes. As the vibration amplitude decreases, lower relative motion between solid particles is observed, leading to a drastic decrease in the damping performance of PDs. In this work a new approach is investigated, in which the damper contains a combination of both solid and liquid fillings, to overcome the shortcomings of a conventional PD. In order to quantify and understand the influence of various dissipation mechanisms, simulations were performed. The liquid motion is modeled using the Smoothed Particle Hydrodynamics (SPH) method and the Discrete Element Method (DEM) is used to model the motion of solid particles. In order to validate the simulation models, also a laboratory experiment was set up. The experimental apparatus consists of a damper, in this case a cylindrical acrylic container filled with spherical particles in combination with a liquid, mounted on a vertical leaf spring. By analyzing the free oscillation behavior of the leaf spring, the corresponding damper performance is characterized. Experimental and simulation results show more relative motion, hence more energy dissipation, in liquid-filled PD case than purely solid filled PD case, especially under low vibration amplitudes. Moreover, numerical studies were performed using a coupled SPH-DEM approach to study the effect of solid particle density and the particle shape on the energy dissipation in liquid filled particle dampers.

Model reduction of second-order systems with MORLAB

Peter Benner (*MPI Magdeburg, Germany*)

14:40

Ines Dorschky (*University Hamburg, Germany*)

Timo Reis (*University Hamburg, Germany*)

Matthias Voigt (*TU Berlin, Germany*)

Steffen Werner (*MPI Magdeburg, Germany*)

We discuss model order reduction (MOR) of second-order systems as they are used to describe the dynamics of mechanical and vibrational systems, and in particular, their response to excitations. A particular focus is on preserving the structure and physical properties of dissipative systems. The discussed algorithms are implemented in the MATLAB and Octave toolbox MORLAB, the Model Order Reduction LABORatory. Numerical experiments are used to illustrate the potentials and limitations of the proposed algorithms.

Global proper orthogonal decomposition for parametric nonlinear model order reduction

Christian H. Meyer (*Technical University of Munich, Germany*)

15:00

Christopher Lerch (*Technical University of Munich, Germany*)

Daniel Jean Rixen (*Technical University of Munich, Germany*)

Finite element simulations of structures that undergo large deformations can imply long simulation times due to the nonlinearity of the resulting equation of motion and a high number of degrees of freedom. Especially for design studies, where the equation of motion must be solved several times, it is highly desired to reduce the simulation time.

The simulation time can be reduced by applying model reduction. Nonlinear model reduction is carried out in two steps: First, the dimension of the problem is reduced by projecting the equation of motion onto a low-order subspace that is defined by a reduction basis. Second, the evaluation of the nonlinear restoring force term, that originates from large deflections, is accelerated through hyperreduction.

The first step can be challenging for systems with large parameter changes. For those systems, the calculated reduction basis must either be updated several times or must provide a subspace that captures the solution vectors for the whole parameter space.

The latter option can be performed by sampling the parameter space, performing full simulations at these sampling points and then applying a proper orthogonal decomposition on the solution vectors.

This contribution shows how this procedure is used for parametric model reduction of geometric nonlinear structures. It also demonstrates its accuracy on a shape-parameterized structure that undergoes large deflections.

Impact of model reduction on frequency responses of linear and geometric nonlinear finite element models

Christopher Lerch (*Technical University of Munich, Germany*)

15:20

Christian H. Meyer (*Technical University of Munich, Germany*)

Boris Lohmann (*Technical University of Munich, Germany*)

Analyzing the behavior of mechanical structures with regard to periodic excitations is an important tool in structural mechanics. Complex structures are typically assembled of multiple components. Thus, the transfer function of an individual component, from one mounting point to another, naturally plays an important role in the overall system behavior. In industrial applications a single component can possess several hundred thousands to millions of degrees of freedom, rendering the calculation of its frequency response functions a challenging task.

When reaching geometric nonlinear behavior due to high excitation levels, such as for lightweight structures, analyses have to be extended to nonlinear frequency response functions. Those are calculated using the shooting method (time-domain) or harmonic balancing (frequency-domain) in combination with a continuation algorithm. The numerical effort for calculation increases drastically with respect to the number of degrees of freedom and excitation levels of interest.

Model reduction aims for resolving this burden. The model is reduced by projecting the equations of motion onto a lower-order subspace, spanned by a reduction basis ideally covering the main dynamics. Thus, a low-order model can be utilized as approximation for the original high-order one. In model reduction of geometric nonlinear systems, the evaluation of the nonlinear internal restoring forces has to be accelerated additionally through hyper reduction.

This work focuses on model reduction of linear and geometric nonlinear mechanical systems concerning a good approximation of the input-output behavior. It starts with reviewing classical model reduction methods for linear mechanical systems and arrives at an approach for systematic extension of the bases for the reduction of geometric nonlinear mechanical systems. The impact of the projection step, meaning the specific choice of reduction basis, is analyzed based on (nonlinear) frequency response functions for various examples.

Parameter variation on nonlinear energy sink attached to multiple degree of freedom system

Martin Jahn (*Leibniz-Universität Hannover, Germany*)

15:40

Lars Panning-von Scheidt (*Leibniz-Universität Hannover, Germany*)

Jörg Wallaschek (*Leibniz-Universität Hannover, Germany*)

The importance of lightweight structures has increased in the last years motivated by the goals of improving efficiency of vehicles and conserving resources. In most cases the loss of weight by using fewer or lighter materials is accompanied by a reduction of the structures stiffness having a strong effect on occurring vibrations. Even if the damping ratio of the structure remains unchanged, by reducing weight and stiffness the vibration amplitudes might increase if the vibration excitation stays the same. Damping elements might be introduced to the structure mitigating critical resonance gains of the structure to reduce these vibrations. In this work the dynamics of a linear multiple degrees of freedom structure with a nonlinear damping element are investigated.

The damping elements are chosen to have a nonlinear characteristic to allow for a situation adaptive design. Numerical parameter studies are carried out to optimize the resulting damping of the entire structure taking into account parameter uncertainties to ensure a robust design. The nonlinear equation of motion is solved by applying the Harmonic Balance Method. The evaluation of the performance of the nonlinear damping element is done by consideration of the nonlinear frequency response functions of the structure. Additional investigation will focus on the consideration of the damping ratios of the nonlinear modes of the structure to evaluate the performance of the damping element.

DFG-PP 1897.02 | Calm, smooth and smart - novel approaches for influencing vibrations by means of deliberately introduced dissipation

Date: February 19, 2019

16:30-18:30

Room: HS 41

Organiser: Peter Eberhard (*University of Stuttgart, Germany*)

Parameter identification of brake pad shims for complex eigenvalue analysis

Dominik Schmid (*Technical University of Berlin, Germany*)

16:30

Vincent Sessner (*Karlsruher Institute of Technology, Germany*)

Nils Gräbner (*Technical University of Berlin, Germany*)

Utz von Wagner (*Technical University of Berlin, Germany*)

Kay A. Weidenmann (*Karlsruher Institute of Technology, Germany*)

Composite structures called shims are bonded on brake pad backplates to increase the damping in brake systems. The aim of this measure is to avoid squeal which is a high-frequent audible brake vibration disturbing the environment. This NVH problem originates from self-excited vibrations resulting from the friction contact between pad and disk. The multi-layer shim compounds consisting of steel and elastomer layers use the shear deformation of the viscoelastic core leading to a high energy dissipation potential.

This contribution focuses on parameter identification for complex eigenvalue analyses. There are two phenomena leading to frequency respectively temperature dependent loss factors. First the viscoelastic behavior of the elastomer layer and second the mode shape dependencies which are related to corresponding natural frequencies. To understand these two phenomena three point bending dynamic mechanical analysis are performed to determine the temperature and frequency dependent viscoelastic properties of the shim structures under continuous forced excitation. The resulting loss factor ($\tan \delta$) will be displayed as a master curve using the time temperature superposition principle. The master curves will be compared with results from experimental modal analysis. The differences between the two procedures are pointed out and the comparability of the results will be discussed. The main goal is to identify input parameters, especially damping characteristics, for subsequent complex eigenvalue analysis.

This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) WA 1427/27-1 "Suppressing brake vibrations by deliberately introduced damping" and WE 4273/16-1 & KA 4224/3-1 "Hybrid CFRP/elastomer/metal laminates containing elastomeric interfaces for deliberate dissipation" within the PP 1897.

On the dynamics of a prestressed sliding wedge damper

Jimmy Aramendiz (*KIT Karlsruhe, Germany*)

16:50

Alexander Fidlín (*KIT Karlsruhe, Germany*)

Eugen Baranowski (*KIT Karlsruhe, Germany*)

The limitation of unwanted oscillations in technical systems is an ever-present task in mechanical engineering. Especially in the resonance regime, the consequences of undesired oscillations can range from mild user discomfort to a total system failure. In order to limit these oscillations, damping is normally introduced into the system. In most applications the introduced damping takes the form of a viscous damping which is always present, thus constantly dissipating energy. The objective of this paper is to investigate a system composed of a simple harmonic oscillator with a prestressed sliding wedge damper attached to it. The damper contains an additional mass and two massless V-form wedges, which are connected by a spring and thus clamp the additional

mass. The chosen system replaces a viscous damping by means of dry friction in combination with the sliding wedges. Because of the dry friction, this damper also offers the additional advantage of sticking, which limits the energy dissipation to the vicinity of the resonance regime. Additionally, the damper offers the practical advantage of being an add-on solution.

First, the nonlinear equations of motions of the proposed two degrees of freedom system are derived and analyzed via averaging methods. Second, the analytical solution is validated by comparing it to a numerical model. In order to model the systems sticking behavior, including the statically indeterminate state, an elastoplastic friction model is chosen. Last, a small parameter study is conducted for chosen parameters.

The analytical and numerical solution show an acceptable agreement within the range of asymptotical methods. However, the derived analytical solution only exists within a given parameter range. The parameter study gives an insight into the effect which each parameter has on the system's dynamics. Additionally, the system shows robustness with respect to the excitation force amplitude, which is a characteristic trademark of viscous damping. This work offers the first insight into the depicted system, proposes two models describing its dynamics, and gives start to further experimental validation.

Acknowledgements

This work has been supported by the DFG German Research Foundation Grant FI 1761/2-1 within the Priority Program SPP 1897 "Calm, Smooth and Smart - Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation".

Application of a variational higher order mixed shell theory towards understanding the deformation behavior of hybrid laminates

Alexander Jackstadt (*Karlsruhe Institute of Technology (KIT), Germany*) 17:10

Wilfried V. Liebig (*Karlsruhe Institute of Technology (KIT), Germany*)

Vincent Sessner (*Karlsruhe Institute of Technology (KIT), Germany*)

Kay A. Weidenmann (*Karlsruhe Institute of Technology (KIT), Germany*)

Luise Kärger (*Karlsruhe Institute of Technology (KIT), Germany*)

Hybrid laminates containing an elastomer layer in addition to fiber reinforced polymer as well as metal layers have been found beneficial in compensating issues frequently found with traditional fiber metal laminates. Commonly used equivalent single-layer shell and plate theories, however, are unable to account for the strong heterogeneous stiffness distribution of the constituents within the laminate. Furthermore, the transverse shear and normal deformations in the elastomer layer are expected to significantly influence the deformation of the neighboring laminae. An accurate depiction of these transverse stresses requires a multi-layer shell theory as opposed to commonly used single-layer formulations. Hence, a higher order mixed variational formulation shell theory is proposed in order to study and predict the mechanical behavior of such laminates, especially on a structural level where the computational effort forbids the use of a three dimensional continuum formulation.

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Identification of radiation damping from modal analysis of structural acoustic systems in unbounded domains

Suhaib Koji Baydoun (*Technische Universität München, Germany*)

17:30

Steffen Marburg (*Technische Universität München, Germany*)

Acoustic radiation damping denotes the energy dissipation of vibrating structures due to sound radiation into the far field. While acoustic radiation damping is rather small and negligible in many engineering applications, it is nevertheless the primary energy dissipating mechanism for lightweight structures with large radiating surfaces. Attempts to reduce the vibrational response of those lightweight structures by additional mechanical damping can only be successful if the extent of mechanical damping is comparable or larger than the extent of radiation damping. In this regard, engineers are in need of reliable and flexible methods for the quantification of radiation damping as well as for the modelling of its effect in an early stage of the design process.

In this paper, the modal radiation loss factors are obtained from an eigenvalue analysis of the coupled structural acoustic system. The equations of time-harmonic elastodynamics and acoustics are addressed by means of finite and boundary element methods respectively. The decoupled, purely structural model subject to acoustic loading is obtained by forming the Schur complement. The nonlinear eigenvalue problem is solved by employing frequency approximations of acoustic impedance matrix. The thereby obtained modes represent the structural modes subject to fluid loading. The modal radiation damping values can be obtained from the complex eigenvalues. The approach is verified based on the example of a honeycomb sandwich panel in air and the results are compared to other numerical as well as to experimental results found in the literature. The method enables researchers to better understand and to quantify the effect of acoustic radiation damping and to estimate its relevance for future research.

Overcoming directional damping limitation - investigation for two degree-of-freedom system

Aditya Suryadi Tan (*Technical University Ilmenau, Germany*)

17:50

Thomas Sattel (*Technical University Ilmenau, Germany*)

Directional damping is a method used to intentionally generate a damping force in a desired direction. In some cases, for example in a positioning task, directional damping is beneficial as a damping force can be generated in the orthogonally to the direction of desired motion while at the same time leaving this direction undamped or minimally damped. By doing so, any unwanted vibrations in any direction other than the positioning direction can be damped while preserving the system dynamics for fast positioning. In an N-Degree-of-Freedom (DoF) movement, where the systems DoF are considered as spatial DoF, an N-number of damping elements are needed to change the resultant damping direction. For this purpose, the damping constant of each damping element needs to be independently adjustable. This kind of adjustment can be realized through the implementation of a field responsive fluid, such as electro- or magnetorheological fluid. Even though the resultant damping direction can be varied, an N-number of damping elements is not enough to realize directional damping in N-DoF, except in the damping axis of the damping element itself. Therefore, an additional adjustable damping element is required to overcome this limitation. In this work, three damping elements are investigated for a two-DoF system. The damping elements each have their own fixed damping axes that are distributed at equal angles around the origin. In order to describe the behavior of the damping system, investigations were conducted for several combinations of damping magnitude and velocity direction. It is shown that with precise adjustment of the damping constant for each damping element, the directional damping can be realized in more than only the damping axis of each damping element.

DFG-PP 1962.01 | Non smooth and complementarity-based distributed parameter systems: simulation and hierarchical optimization

Date: February 19, 2019

14:00-16:00

Room: HS 07

Organiser: Michael Hintermüller (*Weierstraß-Institute Berlin, Germany*)

Structural total variation regularization with applications in inverse problems

Michael Hintermüller (*Weierstraß-Institute Berlin, Germany*)

14:00

We introduce a function space setting for a wide class of structural/weighted total variation (TV) regularization methods motivated by their applications in inverse problems. In particular, we consider a regularizer that is the appropriate lower semi-continuous envelope (relaxation) of a suitable total variation type functional initially dened for siciently smooth functions. We study examples where this relaxation can be expressed explicitly, and we also provide renements for weighted total variation for a wide range of weights. Since an integral characterization of the relaxation in function space is, in general, not always available, we show that, for a rather general linear inverse problems setting, instead of the classical Tikhonov regularization problem, one can equivalently solve a saddle-point problem where no a priori knowledge of an explicit formulation of the structural-TV functional is needed. In particular, motivated by concrete applications, we deduce corresponding results for linear inverse problems with norm and Poisson log-likelihood data discrepancy terms. Finally, we provide proof-of-concept numerical examples where we solve the saddle-point problem for weighted TV-denoising as well as for MR guided PET image reconstruction.

Monotone multilevel method and least-squares finite elements for linear elastic contact

Gabriele Rovi (*Università della Svizzera italiana, Switzerland*)

14:40

Bernhard Kober (*Universität Duisburg-Essen, Germany*)

Gerhard Starke (*Universität Duisburg-Essen, Germany*)

Rolf Krause (*Università della Svizzera italiana, Switzerland*)

We study the first order system least-squares (FOSLS) formulation for the Signorini's problem in linear elasticity and its discretization with mixed finite elements. We then derive efficient multigrid method for the solution of the arising discrete complementarity problem.

Since the formulation is mixed, both primal and dual variables have to be taken care of. In particular the discretization is carried out by continuous piecewise linear functions for the displacement and by the lowest order Raviart-Thomas functions for the stress. Regarding the contact conditions, the linear inequality constraints are embedded in the convex set in which we search for the solution, while the non-linear complementarity term is added to the least-squares functional. In order to solve the discretized problem a monotone multilevel method is used. Indeed we sequentially minimize the energy by solving non-linear local subproblems. In the numerical experiments we show the optimal complexity of the method which holds for both compressible and incompressible materials.

Directional differentiability for parabolic QVIs of obstacle type

Amal Alphonse (*Weierstrass Institute, Germany*)

15:00

Michael Hintermüller (*Weierstrass Institute, Germany, Humboldt-Universität zu Berlin, Germany*)

Carlos N Rautenberg (*Weierstrass Institute, Germany, Humboldt-Universität zu Berlin, Germany*)

In this talk, we consider parabolic quasi-variational inequalities of obstacle type. We first provide an existence result for such QVIs by the method of time discretisation and approximation through elliptic QVIs and then move on to studying differentiability properties of the solution map that takes the source term of the QVI onto the set of solutions. We characterise the derivative as a limit of a monotone sequence of derivatives of parabolic VIs. We shall also point out some alternate approaches to derive the result.

Optimal control of static contact in finite strain elasticity

Anton Schiela (*University of Bayreuth, Germany*)

15:20

Matthias Stöcklein (*University of Bayreuth, Germany*)

Nonlinear elastic problems usually appear in modeling the deformations of nonlinear materials in classical mechanics. These deformations can be described as minimizers of an respective energy functional. In this setting, the resulting optimization problems are highly nonlinear and nonconvex. Extending this to contact problems and an optimal control approach yields a nonsmooth, nonconvex, nonlinear and constrained optimization problem. In order to address this problem analytically and numerically, a suitable regularization is introduced. The focus of the talk lies on the theoretical results we have achieved so far such as existence theory and convergence results for the regularized problems. In addition, we give a numerical analysis on solving these kinds of problems and give an example.

Optimizing fracture propagation using a phase-field approach

Ira Neitzel (*Universität Bonn, Germany*)

15:40

Thomas Wick (*Leibniz Universität Hannover, Germany*)

Winnifried Wollner (*Technische Universität Darmstadt, Germany*)

We consider an optimal control problem of tracking type governed by a time-discrete regularized phase-field fracture or damage propagation model. The energy minimization problem describing the fracture process is described by the corresponding Euler-Lagrange-equations that contain a regularization term that penalizes violation of the irreversibility condition in the evolution of the fracture. We show convergence of solutions of the regularized problem when taking the limit with respect to the penalty term, and obtain an estimate for the constraint violation in terms of the penalty parameter γ . Finally, we show that certain isolated local minimisers of the limit problem can be approximated by this procedure.

DFG-PP 1962.02 | Non smooth and complementarity-based distributed parameter systems: simulation and hierarchical optimization

Date: February 19, 2019

16:30-18:30

Room: HS 07

Organiser: Michael Hintermüller (*Weierstraß-Institute Berlin, Germany*)

Unique global solutions in PDE and VI-constrained optimization

Ahmad Ahmad Ali (*Universität Hamburg, Germany*)

16:30

Klaus Deckelnick (*Otto-von-Guericke Universität Magdeburg, Germany*)

Michael Hinze (*Universität Hamburg, Germany*)

In [1] we consider an optimal control problem subject to a semilinear elliptic PDE together with its variational discretization, where we provide a condition which allows to decide whether a solution of the necessary first order conditions is a global minimum. This condition can be explicitly evaluated at the discrete level. Furthermore, we prove that if this condition holds uniformly with respect to the discretization parameter the sequence of discrete solutions converges to a global solution of the corresponding limit problem. Moreover, in [2] we prove error estimates for those discrete global solutions, which are confirmed by numerical experiments. Our approach can be modified and adapted in order to derive corresponding conditions for the optimal control of the obstacle problem. With this talk we present an overview of our achievements obtained so far.

[1] A.Ahmad Ali, K.Deckelnick, M.Hinze, Global minima for semilinear optimal control problems, *Comput. Optim. Appl.* 65 (2016), 261–288.

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Total variation of the normal as a prior in geometric inverse problems

Roland Herzog (*TU Chemnitz, Germany*)

17:10

Ronny Bergmann (*TU Chemnitz, Germany*)

Marc Herrmann (*University of Würzburg, Germany*)

Stephan Schmidt (*University of Würzburg, Germany*)

Jose Vidal-Nunez (*TU Chemnitz, Germany*)

The total variation (TV) is an important regularizing seminorm in inverse problems and in particular in imaging applications. In this presentation we consider problems where the shape is among the unknowns. We define the notion of total variation of the surface normal as a prior for this class of problems and discuss this term in the continuous and discrete settings. We also address a suitable numerical scheme to deal with the non-smoothness arising from the TV of the normal and present numerical results.

Solving inverse optimal control problems to global optimality

Stephan Dempe (*TU Bergakademie Freiberg, Germany*)

17:30

Felix Harder (*BTU Cottbus-Senftenberg, Germany*)

Patrick Mehlitz (*BTU Cottbus-Senftenberg, Germany*)

Gerd Wachsmuth (*BTU Cottbus-Senftenberg, Germany*)

We consider a class of bilevel optimization problems which can be interpreted as inverse optimal control problems. The lower-level problem is an optimal control problem and it has a convex and

parametrized objective function. The upper-level problem is used to identify the parameters of the lower-level problem. We reformulate the inverse optimal control problem using the optimal value function of the lower-level problem. The feasible set of this reformulation is relaxed by using piecewise affine approximations of the optimal value function. This allows us to compute global optimal solutions of the original non-smooth and non-convex inverse optimal control problem. We investigate both the continuous bilevel problem as well as the discretized problem and present numerical examples.

Structure of subgradients for the obstacle problem and numerical realization

Anne-Therese Rauls (*Technische Universität Darmstadt, Germany*)

17:50

Stefan Ulbrich (*Technische Universität Darmstadt, Germany*)

Various problems in physics, finance and other areas can be expressed in terms of variational inequalities of obstacle type. The presence of such obstacle problems in the constraint set of an optimal control problem results in nonsmoothness of the optimization problem, since the solution operator of the obstacle problem is only directionally differentiable.

In this talk, we discuss the differentiability properties of a general class of obstacle problems and characterize generalized derivatives from the Bouligand subdifferential of the solution operator for the obstacle problem in all points of its domain. The subgradients we obtain are determined by solution operators of Dirichlet problems on the inactive sets. To use the derived subgradients in practice within nonsmooth optimization methods, a discretization of the obstacle problem is necessary. Therefore, only a sequence of inexact solutions of the obstacle problem and, thus, only a sequence of inexact inactive sets is available. We investigate how the respective subgradients can be approximated in this case.

Numerical approximation of rate-independent evolutions

Michael Sievers (*Technical University of Dortmund, Germany*)

18:10

Christian Meyer (*Technical University of Dortmund, Germany*)

We present a discretization of a rate-independent evolution governed by a non-convex energy functional. While standard continuous and piecewise linear finite elements are used for the discretization in space, we employ a tailored local minimization algorithm for the discretization w.r.t. time. It is shown that sequences of discrete solutions converge to so-called parametrized solutions, as the mesh size tends to zero. This solution concept, that also arises via a vanishing viscosity analysis, allows for solutions which are discontinuous in time. A numerical example shows that our algorithm is able to approximate solutions providing a time discontinuity.

DFG-PP 2020.01 | Cyclic deterioration of high-performance concrete in an experimental-virtual lab

Date: February 19, 2019

14:00-16:00

Room: HS 31

Organiser: Ludger Lohaus (*Leibniz University Hannover, Germany*)

Investigation of failure mechanisms in high strength concrete using 3D-XFEM

Rohan Patel (*Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*)

14:00

Stefan Löhnert (*Institute of Mechanics and Shell Structures, Technical University Dresden, Germany*)

High strength concrete, has a significantly different and denser micro-structure compared to normal strength concrete. The properties of the micro-structure which ultimately depends on the manufacturing process, has remarkable influence on overall material behavior. The optimized cementitious materials and binding agents used as ingredients for high strength concrete cement paste are subjected to self-desiccation during the hydration process which leads to shrinkage[1]. This shrinkage process is susceptible to cause micro-cracks potentially leading to a weakened material. Due to the importance of high strength concrete as a modern building material and due to the significant effort to experimentally test different compositions of high strength concrete especially for the prediction of the life time of the concrete under cyclic loads, a computational model for the development of cracks within the microstructure is developed in this work. In order to obtain realistic results, the microstructural geometry used for the simulation model is obtained by means of computer tomography (micro-CT) scans of concrete samples.

To this end, the discrete crack and its propagation within the micro-structure is simulated using the Extended finite element method (XFEM) [2] including inertia effects in 3D in combination with level set techniques. The level set method is useful to track the position of the crack inside the solution domain. The need for a crack propagation criterion for the XFEM is met by a coupled damage model. When a local damage model is used, it exhibits high spurious mesh dependency. Those pathological effects are overcome by a coupled gradient enhanced damage model also simulated using the XFEM. The gradient enhanced damage values are used as propagation criterion as well as for the determination of the crack propagation direction. Once the crack propagates, the update of the crack surface geometry is performed using an advance algorithm for the level sets [3].

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A unified multiscale modelling approach for concrete fatigue with microscale damage-mechanism implementations

Antonio Caggiano (*TU-Darmstadt, Germany*)

14:20

Diego Said Schicchi (*Leibniz-Institut für Werkstofforientierte Technologien - IWT, Bremen, Germany*)

Stefan Harenberg (*Technische Universität Kaiserslautern, Germany*)

Viktoria Malácris-Pfaff (*Karlsruher Institut für Technologie, Germany*)

Matthias Pahn (*Technische Universität Kaiserslautern, Germany*)

Frank Dehn (*Karlsruher Institut für Technologie, Germany*)

Eddie Koenders (*TU-Darmstadt, Germany*)

This paper provides preliminary results of a research study on the fatigue behavior of High-Performance Concrete (HPC). A multi(two)-scale approach for the numerical analysis of HPC specimens subjected to low- and high-cycle fatigue actions will be presented. The multiscale technique is based on a combination of Cellular Automata (CA) [1], to describe the material microstructural properties, and Finite Element (FE) method, to represent the macroscopic response, allowing to consider the effect of the evolving microstructural changes caused by fatigue. More specifically, projected microscopic representative volume elements equipped with a fracture-based model and combined with a continuous inelastic constitutive law that accumulates damages induced by cycle behaviors represents the lower scale. A “plastic-damage” based model for concrete subjected to cyclic loading is developed combining the concept of fracture-energy theories with stiffness degradation, representing the key phenomenon occurring in concrete under cyclic responses [2]. The paper explores the potential of the technique for assessing the fatigue microcracks formation and growth, and their influence on the macroscale behavior. The numerical activities proposed in this paper stem out from the DFG Priority Program 2020 Project "Cyclic Damage Processes in High-Performance Concretes in the Experimental Virtual Lab".

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Description and analysis of pullout behavior of hooked steel fibers embedded in high performance concrete using phase-field modeling

Mangesh Pise (*University of Duisburg-Essen, Germany*)

14:40

Dominik Brands (*University of Duisburg-Essen, Germany*)

Gregor Gebuhr (*Bergische Universität Wuppertal, Germany*)

Mohammad Sahril (*University of Duisburg-Essen, Germany*)

Jörg Schröder (*University of Duisburg-Essen, Germany*)

Steffen Anders (*Bergische Universität Wuppertal, Germany*)

In the recent decades great research effort has been carried out which result to new innovative concrete types such as high performance concrete (HPC). In HPC steel fibers are obligatory to provide sufficient ductility. During fracture the stresses in concrete are transmitted from matrix to the fibers. These fibers restrain the further growth of the crack and contribute to the energy absorption capacity of the concrete, compare [1, 2]. This holds true not only for static but also for cyclic loading. For example [3] shows that steel fibers affect the deterioration characteristics

in cyclic compression. The effects of fibers are even more pronounced in cyclic flexural tests [1]. In this contribution, experimental series of fiber pullout tests are described focusing on the dependency of compressive strength as basis for numerical analysis. The pullout behavior of straight and anchored steel fibers embedded in concrete at various orientation is investigated in [4]. The aim is to examine the pullout behavior of a single steel fiber and its influence on the overall material behavior of HPCs. A continuum phase-field model based on the variational formulation of fracture in elasto-plastic material is implemented in view of the description of the aforementioned phenomena. For brittle to ductile failure criteria for crack propagation proposed by [5] is followed. The predictive capability of the above mentioned model is analyzed in detail by simulating steel fiber reinforced HPC and compared against experimental data.

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Water-induced failure mechanics for concrete: micro-mechanical model, experimental observation and phase-field coupling

Fadi Aldakheel (*Leibniz-Universität Hannover, Germany*)

15:00

Peter Wriggers (*Leibniz-Universität Hannover, Germany*)

A micro-mechanical framework for modeling water-induced damage mechanism of concrete is outlined within this work. Concrete has a highly heterogeneous micro-structure and its composite behavior is very complex. Due to that a various effects must be considered for analyzing failure response at the micro scale, e.g. modeling the solid skeleton, fluid bulk phases and their interaction. For obtaining a deeper understanding of water influence on the concrete at the micro-level, a micro computed tomography (micro-CT) scan has been performed at the Institute of Building Materials Science (IfB) to illustrate the micro-structure geometry and concrete content, which are required to build up the constitutive model and design the numerical simulation, in line with [1]. To this end, a micro-mechanical model is developed for the coupled problem of fluid-saturated heterogeneous porous media at fracture. The modeling of microscopic cracks in porous heterogeneous media can be achieved in a convenient way by recently developed continuum phase field approaches to fracture, which are based on the regularization of sharp crack discontinuities, as outlined in [2,3,4]. This avoids the use of complex discretization methods for crack discontinuities, and can account for complex crack patterns. The numerical examples proposed in this work stem out from the DFG Priority Program SPP 2020 "Cyclic Damage Processes in High-Performance Concretes in the Experimental Virtual Lab".

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Phase-field modeling and simulation of fatigue phenomena in brittle materials

Marreddy Ambati (*Technische Universität Braunschweig, Germany*) 15:20

Pietro Carrara (*Technische Universität Braunschweig, Germany*)

Roberto Alessi (*Università Roma La Sapienza, Italy*)

Laura De Lorenzis (*Technische Universität Braunschweig, Germany*)

Fatigue is a key phenomenon in mechanics, and is a major cause of more than 60% - 75% of structural failures. Despite the significance of the problem, most existing fatigue theories are based on empirical laws that lack of generality and predictive capabilities. Hence, the development of mathematically sound and reliable fatigue models is still an open issue.

A novel variational framework to simulate the fatigue behavior of brittle materials based on the phase-field approach to fracture is presented [1]. The standard regularized free energy functional is modified introducing a fatigue degradation function that reduces the fracture toughness as a proper history variable accumulates as in [2]. The proposed approach aims at linking regularized fracture mechanics to fatigue crack growth, thus establishing a framework suitable for any type of (brittle) materials. The present framework is formulated in the 2- and 3-D setting, allowing to study the major features of the fatigue behavior including crack nucleation, stable and unstable propagation.

Numerical examples show that the Wöhler curve, the crack growth rate curve and the Paris law are naturally reproduced, while the approximate Palmgren-Miner criterion and the monotonic loading conditions are obtained as special cases.

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On the analysis of crack-closure behaviour using the phase-field method together with the novel concept of Representative Crack Elements

Johannes Storm (*Technische Universität Dresden, Germany*) 15:40

Supriatna Dennie (*Technische Universität Dresden, Germany*)

Michael Kaliske (*Technische Universität Dresden, Germany*)

For the analysis of crack closure behaviour and the determination of forces transferred across the crack, several stress-based splits are used for the phase-field method so far. Steinke and Kaliske [2018] proposed a kinematic analysis of the crack-closure behaviour for isotropic linear-elastic material behaviour, which overcomes some important issues of the previous splits (volumetric-deviatoric and spectral split). The talk presents a novel approach for the phase-field method, which adopt the idea of a kinematic crack analysis. Therefore, an underlying representative model of a discrete crack is coupled to the phase-field model in order to determine the degraded and the crack-closure behaviour. Finally, closed solutions of the approach are presented for isotropic and anisotropic, linear elasticity. The model is validated by showing self-consistency and the results are compared to those from the previous mentioned splits.

DFG-PP 2020.02 | Cyclic deterioration of high-performance concrete in an experimental-virtual lab

Date: February 19, 2019

16:30-18:30

Room: HS 31

Organiser: Ludger Lohaus (*Leibniz University Hannover, Germany*)

DEM calibration for modelling of the fatigue behavior of ultra-high-performance concrete

Sebastian Rybczynski (*Hamburg University of Technology, Germany*)

16:30

Maksym Dosta (*Hamburg University of Technology, Germany*)

Frank Schmidt-Doehl (*Hamburg University of Technology, Germany*)

Due to the growing demand for renewable energies, the field of offshore wind turbines is becoming increasingly important. In this area ultra-high-performance concrete (UHPC) is for example used to build high-strength foundations for the pile structure. A similar kind of UHPC is further used in bridge constructions, leading to a reduction of the dead weight and therefore making it possible to build more delicate structures.

As a common feature of both examples, winds, heavy swell or traffic are acting upon the used concrete. Frequent observations of structural defects suggest that these concretes are more susceptible to fatigue than plain concrete leading to an increase of research in this field. The crack initiation from capillary pores can not necessarily be assumed as it is the case in plain concrete. Hence, the aim of this project is to localize the crack initiation, track the crack growth and reproduce the behaviour in discrete element method (DEM) simulations.

For numerical investigations of mechanical behaviour of UHPC the bonded-particle model (BPM) has been used. BPM is an extension of the DEM, where each two primary particles can be connected with solid bonds. This allows to reproduce concrete structure, which contains aggregates and additives embedded into hydrated cement. In this contribution a three-phase model of UHPC, consisting of two types of particles (cement and aggregate particles) and three types of bonds (cement-cement, cement-aggregate, aggregate-aggregate), was modelled. To capture the fatigue behaviour of UHPC, a rheological model containing plastic deformation and weakening has been proposed for the cement-cement bonds.

In order to validate simulations and to estimate unknown model parameters, a set of experimental investigations has been performed. Various load tests on pure cement, aggregate and UHPC samples were carried out in order to obtain material characteristics. Additionally, to maintain realistic non-spherical shape of the aggregates μ -CT analysis have been used.

Characterizing high performance concrete in the frequency domain: validation experiments

Josef Sauer (*University of Stuttgart, Germany*)

16:50

Jana Musialak (*Ruhr-Universität Bochum, Germany*)

Holger Steeb (*University of Stuttgart, Germany*)

High Performance Concrete (HPC) and Ultra High Performance Concrete (UHPC) respectively achieve an effective stiffness or strength reaching or even exceeding that of metal, allowing for buildings which are extremely slender, e.g. offshore windparks or bridges. At the same time, the effective material properties depend on environmental conditions like humidity and on material inherent micro- and meso-scale imperfections like fractures. Following, we present a novel characterization technique for HPC and UHPC, using harmonic excitations from 0.1 Hz

up to 1 kHz and displacement amplitudes in the micrometer range. The excitations will be performed by a high-performance piezo-electric actuator. Through the experimental characterization, frequency-dependent complex moduli of HPC/UHPC samples are determined via a Fast Fourier Transformation, based on the local strains measured by strain gauges. A long-term goal is the observation of crack initiation and growth, as well as observing the influence of humidity on these phenomena.

To validate the experimental workflow, we characterize the mechanical behaviour of Polymethylmethacrylat (PMMA). PMMA is known for its effective viscoelastic behaviour, which makes it highly useful for fundamental rheological investigations.

In this contribution, we present results gained with two different cylindrical sample sizes. By this comparison we shall ensure that geometrical scaling of samples has no influence on the rheological results of the experiments, apart from a change in Signal-to-Noise ratio. Such, we make way for future experiments with miniature samples of HPC and UHPC, which will be easier to fracture and to integrate into set-ups for X-Ray Computed Tomography (XRCT).

Influence of load-induced temperature on fatigue behaviour of UHPC

Ngoc Linh Tran (*Technische Universität Darmstadt, Germany*)

17:10

Melchior Deutscher (*Technische Universität Dresden, Germany*)

Silke Scheerer (*Technische Universität Dresden, Germany*)

Recent experimental works on concrete fatigue show that there is a significant increase of load-induced temperature in ultra-high performance concrete, especially by high loading rates. The temperature field is not uniformly distributed in concrete which causes constrained stresses and leads to a reduction of concrete fatigue strength. Two issues to be examined are the mechanism of heat-generation in concrete due to cyclic loading and the influence of load-induced temperature on the fatigue behaviour of concrete. In this paper, new formulations of the development of strain and stress due to cyclic loadings are presented, in which a fatigue failure criterion based on critical strains is proposed. Besides the elastic, creep and thermal strains, the damage strain is of particular interest. The influences of the load frequency and the maximum size of aggregate of concrete on the temperature development and on the fatigue behaviour of concrete are also taken into account. The theoretical formulations are validated and calibrated on the basis of existing experimental results, including the experimental works carried out by the authors. Discussions on the development of load-induced temperature and fatigue damage of concrete are also presented.

Poster Session

Date: February 19, 2019 16:00-16:30
Room: Kleiner Festsaal
Organiser: Rafael Reisenhofer (*University of Vienna, Austria*)

Information about the GAMM student chapter Chemnitz

Alexandra Buenger (*Technical University Chemnitz, Germany*)

The GAMM Student Chapter Chemnitz was founded immediately after the GAMM board introduced student chapters in 2015. Since its formation we organized numerous events to promote the interdisciplinary exchange between Master and PhD students of applied mathematics and mechanics at the Technical University Chemnitz.

This poster presents an overview of our chapter's scientific and social activities during the last year.

A phase mixture model for martensitic steels

Johanna Eisenträger (*Otto von Guericke University Magdeburg, Germany*)

Tempered martensitic steels are established materials for components used in power plants at high temperatures up to 903 K. Due to the high temperatures prevailing and frequent start and stop operations of power plants, the mechanical behavior of the components is affected by creep as well as fatigue. However, martensitic steels offer excellent thermo-mechanical properties to withstand these challenging conditions. On the other hand, these alloys tend to soften under constant and cyclic loads.

This contribution presents a phase mixture model to simulate the mechanical behavior of these components. By employing an iso-strain approach with a soft and a hard constituent, the model accounts for rate-dependent inelasticity, hardening, as well as softening effects. While the hard constituent comprises the subgrain boundaries and areas with a high dislocation density, the soft constituent represents the interior of the subgrains and regions with a low dislocation density. The model incorporates two internal variables, i.e. a backstress of Armstrong-Frederick type and a dimensionless softening variable, and results in a system of three evolution equations for the inelastic strain, the backstress, and the softening variable.

Within a complex calibration procedure, all required material parameters are determined based on high temperature tensile and creep tests. This results in a set of 16 parameters, which are required to simulate the mechanical behavior of martensitic steels with respect to wide ranges of temperature and stress, i.e. 673-923 K and 100-700 MPa. In order to allow for the analysis of real power plant components, the phase mixture model is implemented into the finite element code ABAQUS using a user material subroutine (UMAT). The evolution equations are integrated with respect to time based on the backward Euler method. Furthermore, the consistent tangent operator is derived analytically, and the implementation of the model into the finite element method is verified by several benchmarks, covering both uniaxial and multiaxial stress and deformation states.

Mixed frameworks and structure preserving integration for coupled electro-elastodynamics

Marlon Franke (*Karlsruhe Institute of Technology, Germany*)

Rogelio Ortigosa (*Polytechnic University of Cartagena, Spain*)

Alexander Janz (*Karlsruhe Institute of Technology, Germany*)

Antonio J. Gil (*Swansea University, United Kingdom*)

Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

An identical contribution is included at Section S04: Structural mechanics. Please see the respective section for the related abstract.

Topology and shape optimization with application to electrical machines

Peter Gangl (*Technische Universität Graz, Austria*)

This poster deals with the task of finding the optimal design for an electric motor by means of topology and shape optimization. The problem can be formulated as a shape optimization problem which is constrained by the quasilinear partial differential equation (PDE) of two-dimensional nonlinear magnetostatics.

In a first stage, we derived the topological derivative for the problem at hand and use this sensitivity information in an optimization algorithm using a level set representation of the domain. The topological derivative for the problem involving a quasilinear PDE constraint is the sum of two terms. Here, the efficient numerical evaluation of the second term, which would vanish in the case of a linear PDE constraint, is particularly challenging.

In a second stage, we perform shape optimization based on the shape derivative of the quasilinear problem at hand as a post-processing step. Here, the accurate resolution of the material interface between ferromagnetic material and air regions is considered by means of a local mesh modification strategy.

We illustrate the algorithms by applying them to a model problem from electrical engineering. Moreover, we introduce a multi-material topology optimization algorithm based on the topological derivative. Here, we extend the topology optimization algorithm from two different materials (ferromagnetic material and air) to the case of three materials (e.g. ferromagnetic material, air and permanent magnet).

Sparse recovery from superimposed non-linear measurements

Martin Genzel (*Technische Universität Berlin, Germany*)

In this presentation, we study the problem of sparse recovery from superimposed, non-linearly distorted measurements. This challenge is particularly relevant to wireless sensor networks that consist of autonomous and spatially distributed sensor units. Here, each of the M wireless sensors acquires m individual measurements of an s -sparse source vector. All devices transmit simultaneously to a central receiver, causing collisions. Since this process is imperfect, e.g., caused by low-quality sensors and the wireless channel, the receiver measures a superposition of corrupted signals. First, we will show that the source vector can be successfully recovered from $m = O(s \log(2n/s))$ coherently communicated measurements via the vanilla Lasso. The more general situation of non-coherent communication can be approximated by a bilinear compressed sensing problem. Even in the non-linear setting, it will turn out that $m = O(s \max M, \log(2n/s))$ measurements are already sufficient for reconstruction using the Group-Lasso. In particular, as long as $M = O(\log(2n/s))$ sensors are used, there is no substantial increase in performance when building a coherently communicating network. Finally, we discuss several practical implications and extensions of our approach. This is joint work with Peter Jung (TU Berlin).

Adaptivity in model order reduction with proper orthogonal decomposition

Carmen Gräßle (*Universität Hamburg, Germany*)

Michael Hinze (*Universität Hamburg, Germany*)

We consider the approximation of dynamical systems with model order reduction based on Proper Orthogonal Decomposition (POD). The basic idea is to replace high-fidelity solutions by low dimensional approximations utilizing a POD Galerkin approach.

A crucial challenge within snapshot-based POD model order reduction for time-dependent systems lies in the input dependency. In the 'offline phase', the POD basis is computed from snapshot data obtained by solving the high-fidelity model at several time instances. If a dynamical structure is not captured by the snapshots, this feature will be missing in the ROM solution. Thus, the quality of the POD approximation can only ever be as good as the input material. In this sense, the accuracy of the POD surrogate solution is restricted by how well the snapshots represent the underlying dynamical system.

If one restricts the snapshot sampling process to uniform and static discretizations, this may lead to very fine resolutions and thus large-scale systems which are expensive to solve or even can not be realized numerically. Therefore, offline adaptation strategies are introduced which aim to filter out the key dynamics. On the one hand, snapshot location strategies detect suitable time instances at which the snapshots shall be generated. On the other hand, adaptivity with respect to space enables us to resolve important structures within the spatial domain. Motivated from an infinite-dimensional perspective, we explain how POD in Hilbert spaces can be implemented. The advantage of this approach is that it only requires the snapshots to lie in a common Hilbert space. This results in a great flexibility concerning the actual discretization technique, such that we even can consider r-adaptive snapshots or a blend of snapshots stemming from different discretization methods. Moreover, in the context of optimal control problems adaptive strategies are crucial in order to adjust the POD model according to the current optimization iterate. In the context of incompressible flows with space-adapted snapshots a further challenge of deriving stable reduced-order models arises. We propose two solution approaches and compare them numerically.

Structural and material optimization based on thermodynamic principles

Dustin Roman Jantos (*Institute of Mechanics of Materials, Ruhr-Universität Bochum, Germany*)

Klaus Hackl (*Institute of Mechanics of Materials, Ruhr-Universität Bochum, Germany*)

Philipp Junker (*Institute of Mechanics of Materials, Ruhr-Universität Bochum, Germany*)

An identical contribution is included at Section S16: Optimization. Please see the respective section for the related abstract.

On symmetry group evolution in finite plasticity

Tobias Kaiser (*TU Dortmund University, Germany*)

Andreas Menzel (*TU Dortmund University, Germany, Lund University, Sweden*)

Jia Lu (*The University of Iowa, USA*)

Panayiotis Papadopoulos (*University of California, Berkeley, USA*)

Motivated by the experimental investigations by Kim and Yin (J. Mech. Phys. Solids 45(5) (1997), 841-851) on the evolution of plastic anisotropies in cold rolled sheet metal, this contribution focusses on the modelling of evolving material symmetry groups in finite strain plasticity. The experiments suggest that the initially orthotropic structure of the yield function's symmetry group that was induced by the rolling process is maintained. However, a rotation of the preferred material axes is observed such that the preferred material directions align with the loading- and with the transverse direction in uniaxial tension tests.

Taking into account the experimental investigations by Kim and Yin, a specific thermodynamically consistent model is proposed which relies on the fundamental theoretical developments in the context of evolving material symmetries in finite strain plasticity reported in (Comput. Methods in Appl. Mech. Eng. 190(37-38) 2001, 4889-4910) and (Comput. Methods in Appl. Mech. Eng. 193(48-51)(2004), 5339-5358). To capture the symmetry group evolution, evolution equations for the structural tensors which characterise the respective material symmetry groups and which are introduced as additional arguments of the yield function, are derived.

A comparison of finite element based simulation results with the experimental findings finally shows the capability of the model in reproducing the experimentally observed texture evolution.

The condensed method: an efficient approach to investigate constitutive behaviors, phase transitions and high-cycle fatigue of polycrystalline ferroelectric, ferromagnetic or multiferroic materials

Stephan Lange (*University of Kassel, Germany*)

Andreas Warkentin (*University of Kassel, Germany*)

Philip Uckermann (*University of Kassel, Germany*)

Marius Wingen (*University of Kassel, Germany*)

Andreas Ricoeur (*University of Kassel, Germany*)

Ferroelectric as well as ferromagnetic materials are widely used in smart structures and devices as actuators, sensors etc. To model their nonlinear behavior, a variety of models has been published in the past decades, e.g. [1]. Most of the models that have been developed were implemented within the framework of the Finite Element Method (FEM), e.g. [2,3,4]. The implementation of a discretization scheme is going along with a high computational effort and the solution of the boundary value problem (BVP) requires high computational costs. Most investigations, however, are restricted to simple BVP under uniaxial or biaxial loading and their goal is the calculation of hysteresis loops or to investigate e. g. electromechanical or magnetoelectric coupling effects. In [5] the so-called condensed method (CM) is introduced to investigate the polycrystalline material behavior at a macroscopic material point without any kind of discretization scheme. In this paper an overview on the CM and its great potential is given. Besides classical ferroelectrics, other fields of application of the CM have been exploited, e.g. ferromagnets, ferroelectric-ferromagnetic composites and ferroelectrics with phase transition [6,7]. Furthermore, based on the condensed theory, a high cycle fatigue model is introduced in [8] to predict the life time of ferroelectric materials under combined electromechanical loading. The latest topic in this field is

the extension of the CM towards nonlinear thermoelectromechanical behavior. Here, the heating of a ferroelectric material, as a result of the irreversible domain wall motion, is investigated.

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A multiscale model of processes in the human liver

Lena Lambers (*University of Stuttgart, Germany*)

Tim Ricken (*University of Stuttgart, Germany*)

Matthias König (*Humboldt University Berlin, Germany*)

The liver is the central metabolic organ of our body, responsible for essential functions like glucose homeostasis or detoxification of drugs from the blood. The metabolic processes are perfusion-dependent and can be influenced by liver diseases.

Since the liver has a complex and hierarchical organized structure, a scale bridging approach is required to understand the interplay between perfusion, metabolism and tissue structure. We have developed a multicomponent, poro-elastic multiphasic and multiscale function-perfusion model based on the Theory of Porous Media (TPM, see [1], [2]). The multiscale approach considers the different functional units of the liver, the so-called liver lobules with an anisotropic blood flow via the sinusoids (slender capillaries between the periportal field and the central vein), cf [3]. We use a multicomponent mixture theory based on the TPM to describe the complex liver micro-structure.

The computational model consists of a tetra-phasic body, composed of a porous solid structure representing healthy tissue, necrotic tissue, resulting from an overdose of toxic metabolites, a liquid phase representing the blood and a fat phase. The latter has ability of growth and depletion during a non-alcoholic fatty liver disease (NAFLD).

The phases consist of a carrier phase, called solvent, and solutes, representing microscopic components e.g. nutrients or paracetamol, dissolved in the solvent.

The hepatic metabolic processes are performed by liver cells, called hepatocytes, which are located along the sinusoids. To calculate these processes and to describe the production, utilization and storage of the metabolites on cellular scale, a bi-scale PDE-ODE approach with embedded coupled ordinary differential equations (ODE) is used.

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Optimal inflow control in supply systems with uncertain demands

Simone Göttlich (*University of Mannheim, Germany*)

Ralf Korn (*TU Kaiserslautern, Germany*)

Kerstin Lux (*University of Mannheim, Germany*)

This poster addresses a stochastic optimal control framework including uncertain demands. In the context of supply chain management, suitable control strategies under uncertainty are necessary for production planning as the size and timing of product orders is often not known in advance. We model this uncertain demand stream by an Ornstein-Uhlenbeck process with an additional jump component. A hyperbolic transport equation describes the dynamics of the supply system.

We present different control approaches to optimally meet the stochastic demand. We come up with an analytical expression of the optimal inflow control for different levels of available demand information. Furthermore, we reformulate the original problem in a way such that classical optimization solvers can be used and compare the different control approaches to each other in a numerical simulation study.

History of logarithmic strain measures in nonlinear elasticity

Robert J. Martin (*Universität Duisburg-Essen, Germany*)

Patrizio Neff (*Universität Duisburg-Essen, Germany*)

Ingo Münch (*Karlsruhe Institute of Technology, Germany*)

Bernhard Eidel (*Universität Siegen*)

Historically, there have been a number of different motivations for the use of logarithmic strain measures in nonlinear elasticity, dating back to the end of the 19th century. Today, the first practical applications of logarithmic strain are often attributed to P. Ludwik (for example in Truesdell's Classical Field Theories), who first mentioned logarithmic strain for uniaxial plastic deformations in his 1909 monograph *Elemente der technologischen Mechanik*. A fully three-dimensional logarithmic elastic law, widely considered to be the first of its kind, was introduced by Heinrich Hencky in his 1928 article *Über die Form des Elastizitätsgesetzes bei ideal elastischen Stoffen*.

However, the first known introduction of the logarithmic strain tensor to fully three-dimensional nonlinear elasticity is actually due to the famous geologist George Ferdinand Becker. In his 1893 article *The Finite Elastic Stress-Strain Function*, he proposed a linear relation between the (material) logarithmic strain tensor and the Biot stress tensor, using a systematic approach remarkably similar to Hencky's. Although it was reviewed in *Beiblätter zu Wiedemanns Annalen der Physik* and cited in Lueger's *Lexikon der gesamten Technik*, Becker's work seems to have gone unnoticed in continuum mechanics until its recent rediscovery. The introduction of the logarithmic strain to elasticity theory is therefore currently misattributed in the literature.

Model order reduction of multi-agent systems

Petar Mlinarić (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Multi-agent systems are network systems where the subsystems, called agents, all have the same dynamics. In particular, we consider multi-agents systems where the agents are linear time-invariant systems, interconnected linearly and diffusively through their inputs and outputs. There are two complementary approaches for structure-preserving model order reduction of such systems: clustering and subsystem reduction. For clustering-based model order reduction, we propose an H2-suboptimal method, combining the iterative rational Krylov algorithm and the k-means clustering algorithm. We motivate the method and compare it to other methods proposed in the literature. For subsystem reduction, we derive necessary optimality conditions for H2-optimal structure-preserving model order reduction and discuss possible solution methods.

Unstructured T-splines based on local higher-dimensional mesh representations

Philipp Morgenstern (*Leibniz Universität Hannover, Germany*)

Roland Maier (*Universität Augsburg, Germany*)

An identical contribution is included at Section S18: Numerical methods of differential equations. Please see the respective section for the related abstract.

Blood damage estimation for medical device design

Lutz Pauli (*RWTH Aachen University, Germany*)

Stefan Haßler (*RWTH Aachen University, Germany*)

Marek Behr (*RWTH Aachen University, Germany*)

Ventricular assist devices (VADs) are used to provide mechanical circulatory support to chronically ill heart disease patients. Even though the devices improved significantly over the last decade, clinical studies still reveal high rates of adverse events associated with the blood damage caused by these devices.

To improve the virtual design of VADs and other blood-handling devices, we developed an Eulerian, strain-based hemolysis model for the quantification of mechanical blood damage and the identification of critical regions within the device. In contrast to commonly used stress-based models, our strain-based model estimates the distortion of red blood cells in the flow field, which allows to consider time-dependent and viscoelastic deformation. Comparisons of stress-based and strain-based hemolysis models in a benchmark blood pump show very significant differences. Stress peaks with short exposure time contribute to the overall hemolysis in the stress-based model, whereas regions with increased shear and long exposure time are responsible for damage in the strain-based model [1].

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Multiscale modeling of dual phase steels

Lisa Scheunemann (*Universität Duisburg-Essen, Germany*)

In modern engineering applications involving dual-phase (DP) steels, detailed knowledge on the material's yield behavior is required, e.g. in the design of forming processes. In DP steel, the microstructure consisting of martensitic inclusions embedded in a ferritic matrix along with the nonlinear behavior of each phase itself contribute to the highly complex macroscopic material behavior. A description based on macroscopic phenomenological material laws is cumbersome and neglects the microscopic origin of many effects. Multiscale methods, such as the FE² method, have been shown to be appropriate approaches to capture these effects. The classical phenomenological material law is replaced by the solution of a microscopic boundary value problem, which consists of a representative volume element (RVE) to represent the microstructure. It is attached at every macroscopic integration point whereas the macroscopic quantities are computed by suitable volume averages over the RVE.

In order to reduce the huge computational effort involved in multiscale computations, the use of statistically similar RVEs (SSRVEs) have been shown to lead to good results. This alternative approach on the microscale level reduces the complexity introduced by RVEs based on real microstructures. SSRVEs are obtained in an optimization process such that the statistical properties of the underlying microstructure of the SSRVE are similar to the ones measured in the real microstructure. The performance of the SSRVE strongly depends on the choice of statistical measures used in the construction as well as the parameterization of the microstructure of the SSRVE. Another important aspect in the accurate description of the material behavior of each individual phase. Single crystal plasticity can be used to describe the elastoplastic behavior, where each grain with a distinct orientation of the atomic lattice is treated separately. Different approaches have been established in this field: In rate-independent models, the set of active slip systems in the grain is possibly nonunique and is identified in, e.g., an active set search. Rate dependent approaches are based on power-type creep laws which do not differentiate into active or inactive slip systems. However, the constitutive equations of these formulations are often very stiff and require a small time increment. Here, a new algorithm for the solution of the constrained optimization problem based on the primal dual interior point method (PDIPM), involving slack variables is presented for the framework of small strain single crystal plasticity. All slip systems are considered simultaneously, omitting an iterative active set search.

Structure-preserving model reduction for the advection-diffusion equation

Philipp Schulze (*TU Berlin, Germany*)

We consider the problem of finding a low-dimensional model for the parameter-dependent linear advection-diffusion equation with Dirichlet-Neumann boundary conditions. Next to the desired computational speedup, the special focus is on preserving the important system properties stability and passivity. Classical model order reduction methods are known to be ineffective for systems where high gradient structures, like shock waves, are advected without experiencing a significant change due to diffusion. Recently, new model order reduction methods have been proposed which are able to obtain reasonable low-dimensional models even for these advection-dominated problems by explicitly taking into account the advection in the approximation ansatz. However, in general they may yield reduced-order models (ROMs) which are neither stable nor passive.

On this poster, we present a new model reduction framework, which is based on the recently introduced shifted proper orthogonal decomposition (shifted POD). Applying this framework to the advection-diffusion equation, we obtain low-dimensional models which preserve stability and

passivity. This is achieved by formulating the full-order model as a port-Hamiltonian system and ensuring the preservation of the port-Hamiltonian structure in the ROM. The numerical results reveal that the shifted-POD-ROM achieves the same accuracy as a standard POD-Galerkin-ROM but with significantly smaller state space dimension. This difference is very much dependent on the diffusion parameter as the difference is only significant in the advection-dominated regime, whereas the POD and the shifted POD perform similarly for the case of large diffusion parameters.

Data-driven modeling of systems with prescribed structure

Benjamin Unger (*Technische Universität Berlin, Germany*)

The dynamics of complex dynamical processes are often analyzed through simulation of an appropriate model of (partial) differential-algebraic equations. Thus, the main cost associated with such an approach is governed by developing an appropriate model and solving the usually high-dimensional model numerically. A remedy for the high or even unmanageable computational burden is model order reduction (MOR), which allows reducing the state space dimension of the high-dimensional system of ordinary differential equations while maintaining good accuracy. The modeling cost can be reduced considerably if the model is built using a purely data-driven approach such as dynamic mode decomposition, the Loewner framework, or Vector Fitting. Although the model constructed from data only, it should still reflect specific physical properties like the preservation of energy, stability, or encode transport phenomena via state delays. In this poster, we present two methods that allow building a low-dimensional realization with a prescribed system structure using only time-domain measurements of the system. The presented results are based on joint work with Riccardo Morandin, Volker Mehrmann, and Philipp Schulze (all TU Berlin).

Shape optimization in shape spaces

Kathrin Welker (*HSU/UniBw Hamburg, Germany*)

The theory of shape optimization is connected to the differential-geometric structure of shape spaces. In particular, efficient algorithms in terms of shape spaces are presented. A constrained shape optimization problem is treated from an analytical and numerical point of view. Shape optimization problems constrained by partial differential equations or variational inequalities are very challenging because of the necessity to operate in inherently non-linear and non-convex shape spaces.

Sections

S01 | Multi-body dynamics

Organiser: Michael Krommer (*Technische Universität Wien, Austria*)
Johannes Gerstmayr (*University of Innsbruck, Austria*)

S01.01 | Multi-body dynamics

Date: February 20, 2019

14:00-16:00

Room: SR 06

Multibody modelling and experimental identification of wind turbines

Christoph Woernle (*University of Rostock, Germany*)

14:00

Roman Rachholz (*University of Rostock, Germany*)

Andreas Schulze (*University of Rostock, Germany*)

Johannes Luthe (*University of Rostock, Germany*)

János Zierath (*W2E Wind to Energy GmbH, Germany*)

Wind turbines are subject to high dynamic loads over their life cycle. The dynamic behaviour is governed by the interaction between structural components like tower and blades, driveline, highly fluctuating aerodynamic loads and plant controller. Co-simulations comprising a flexible multibody model of the mechanical components, an aerodynamic model and controller software prove to be able to predict well the operating behaviour and component loads of wind turbines under nominal conditions and during failure cases.

To validate simulated interface loads under operational conditions, 2 MW and 3 MW prototypes were equipped with strain gauges at specific locations like at the blade root, along the tower or at the low-speed shaft. In addition the actual wind conditions were recorded by a measurement mast in front of the turbine. Using the same controller software in the co-simulations as implemented on the wind turbines provides a good agreement between simulated and measured operating behaviour. This enables a direct validation of simulated interface loads by measurements with generally good agreements.

Further experimental validations of the multibody models were conducted with respect to the modal parameters of the wind turbines. Both classical modal analysis (CMA) and operational modal analysis (OMA) were applied. For wind turbines CMA is only feasible for individual structural components as it is not possible to apply defined test loads on an entire wind turbine. Accordingly CMA analyses were conducted for an individual rotor blade while the rotor was lying on the ground during assembly of the turbine. OMA analyses exploit system output measurements only under the assumption of broadband ambient excitation. Both for the individual rotor blade and for the entire wind turbine OMA was applied using sensor configurations comprising accelerometers and partly additional gyros. Experimental and simulation results are compared with respect to natural frequencies and mode shapes.

Measurements on multi-megawatt wind turbines by means of OMA are expensive, as they are time consuming and require downtimes. Therefore a dynamically scaled wind turbine test rig was developed for testing measurement procedures in the laboratory. The test rig is designed in such a manner that its lower natural frequencies are in the same range as those of real wind turbines. A wireless data acquisition system enables simultaneous measurements on rotating and non-rotating structural components. Ambient draught in the laboratory proved to be sufficient for sound OMA analyses. Results from OMA analyses are compared with numerical simulations based on a detailed flexible multibody model.

Double magnus type wind turbine

Liubov Klimina (*Lomonosov Moscow State University, Russian Federation*) 14:40
Ekaterina Shalimova (*Lomonosov Moscow State University, Russian Federation*)
Marat Dosaev (*Lomonosov Moscow State University, Russian Federation*)
Yury Selyutskiy (*Lomonosov Moscow State University, Russian Federation*)

A closed dynamic model of a counter-rotating Magnus type wind turbine is constructed. The system consists of two propellers with coaxial central shafts. The central shafts are oriented along the flow direction. Several Savonius rotors are connected to the central shaft by cylindrical joints. The axes of these joints are orthogonal to the flow direction. Self-induced rotation of Savonius rotors produces the Magnus force that causes the rotation of the propellers in opposite directions. It is supposed that one of the propellers carries a rotor of an electric generator, and the other one carries a stator of the generator. The generator is connected into a local electric circuit. Aerodynamic torques acting upon the propellers are described using a quasi-steady approach. Stationary modes of such system are studied. The dependence of the trapped power coefficient on the external resistance in the electric circuit is described.

This work was supported by the State Assignment (No. AAAA-A16-116021110197-8)

On grasp based objectives in human grasping simulation

Uday Dattaram Phutane (*FAU Erlangen-Nuremberg, Germany*) 15:00
Michael Roller (*Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM), Germany*)
Sigrid Leyendecker (*FAU Erlangen-Nuremberg, Germany*)

Grasping is a complex human activity performed with the hand via its complicated kinematic and dynamic nature. The dexterity properties of human hand make it a difficult problem to simulate and replicate to human perfection. To evaluate and recreate good grasp postures in simulation and practice, researchers normally employ grasp quality measures. This is an extensive research area due to its applications and utility in areas such as activities of daily living, anthropomorphic robotic systems, industrial tool use etc. We attempt to reproduce human power and precision grasps by employing a kinematically versatile model of the human hand, actuated by joint torques. We have shown the applicability of such a model to perform two finger precision grasps by conceptualizing the grasping action as an optimal control problem (ocp) using the paradigm of discrete mechanics and optimal control with constraints (DMOCC). Solving the ocp (essentially a constrained optimization problem after direct transcription) results in the evolution profiles for configurations, actuation torques, contact forces and also determines contact points on the object surfaces, with regard to specific kinematic and dynamic objectives for grasping motion. The grasping DMOCC setup is extended to compare grasp performance with respect to grasp quality measures, procured from grasp matrix and hand Jacobian mathematical concepts. The grasp quality measures, either individually or as a combination in a weighted sum, act as objective functions. We also compare the effect of hard and soft contact models on grasp performance.

The Influence of foot geometry on the energy efficiency of models for bipedal walking

Ulrich J. Römer (*Karlsruhe Institute of Technology, Germany*) 15:20
Alexander Fidlin (*Karlsruhe Institute of Technology, Germany*)
Wolfgang Seemann (*Karlsruhe Institute of Technology, Germany*)

Bipedal walking was and is an active area of research in the fields of biomechanics and robotics. A fundamental principle of bipedal walking movements is the maximization of energy efficiency. For the analysis, optimization and control of walking movements, a large number of models of very different complexity are being used. In models with low complexity, the feet are often neglected because they have a comparatively low mass and size.

We compare multibody models of bipedal walkers with low or medium complexity with and without feet to quantify the influence of feet on energy efficiency. The models are controlled by the hybrid zero dynamics (HZD) approach which makes use of the models' natural dynamics to swing the legs and achieve a walking movement. The movement as well as the foot geometry are optimized for energy efficiency.

We find that feet have an important influence on energy efficiency in bipedal walking. Models with human-like feet achieve more than twice the energy efficiency when compared to models without feet. Optimization of the foot geometry allows for further significant enhancements.

Biomechanical simulations with dynamic muscle paths on NURBS surfaces

Johann Penner (*University of Erlangen-Nuremberg, Germany*)

15:40

Sigrid Leyendecker (*University of Erlangen-Nuremberg, Germany*)

When simulating musculoskeletal motion with multibody systems representing bones and joints, the muscle paths define the muscle forces, moment arms and resulting body and joint loads. Typically, muscle paths cannot be adequately represented as straight lines because the anatomical structure of the human body forces the muscles to wrap around bones and adjacent tissue. Assuming that the muscles and tendons are always under tension, their path is often modelled as a locally length minimizing curve that wraps smoothly over adjacent obstacles [1,3,4].

The major contribution of this work lies in the use of discrete variational calculus [2] to describe the entire musculoskeletal system, including the muscle paths in a holistic way [3]. Due to the complex geometry of bones and tissue and the fact that muscles can wrap around multiple surfaces, the determination of muscle paths is very challenging. We therefore use non-uniform rational B-spline (NURBS) surfaces to describe the wrapping surfaces and define the muscle paths as a G1-continuous combination of adjacent geodesics [3,4]. In the resulting coupled musculoskeletal system, the muscle path problem is a boundary value problem on free-form parametric surfaces.

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S01.02 | Multi-body dynamics

Date: February 20, 2019

16:30-18:30

Room: SR 06

Improved initialization schemes for the time integration of constrained systems

Martin Arnold (*Martin Luther University Halle-Wittenberg, Germany*)

16:30

The equations of motion of constrained mechanical systems form a differential-algebraic equation (DAE) of index 3. One of the standard approaches in time integration is based on the direct application of stiff ODE integrators to these higher index DAEs. The numerical solution will typically satisfy the original (holonomic) constraint equations with high accuracy but shows a systematic deviation from the manifold that is defined by hidden constraints being obtained by differentiation of the original constraints with respect to time.

Consistent initial values of the analytical solution comply with all the original and hidden constraints in the DAE and do not share the systematic deviation of the numerical solution from hidden constraint manifolds. Therefore, some correction terms need to be added if these (analytically) consistent initial values are used for the initialization of the numerical solution since otherwise large transient error terms and order reduction may be observed in some of the solution components.

In the talk, we will discuss such improved initialization schemes for BDF and for generalized- α methods being applied to constrained systems on linear spaces. Similar results are obtained for systems with nonlinear configuration spaces having a Lie group structure.

A formulation for the dynamic analysis of multibody systems using non-redundant unified local velocity coordinates

Stefan Holzinger (*University of Innsbruck, Austria*)

16:50

Johannes Gerstmayr (*University of Innsbruck, Austria*)

In this paper, we present a formulation for the dynamic analysis of a multibody system using non-redundant unified local velocity coordinates. The motivation for the present work is the result of an earlier investigation of unified local velocity coordinates of Holzinger et al. [5th IMSD, 2018]. The equations of motion presented by the authors are free of rotation parameters and allow the description of the rigid body motion in space by purely translational local velocity coordinates. However, the earlier investigations are limited to the description of the spatial motion of a free rigid body. Therefore, constraints are incorporated in the present paper.

As in the earlier investigations, we limit ourselves in this work to rigid bodies. The linear relationship between Lie algebra and unified velocity coordinates allows to represent the constraint equations at velocity level in terms of unified velocity coordinates. This enables us to add constraint forces to the equations of motion using the method of Lagrange multipliers and therefore to obtain a multibody dynamic formulation with index-2. In earlier studies on the unified local velocity coordinates, the equations of motion and the kinematic reconstruction equations for free rigid body motion were integrated using an explicit fourth-order Runge-Kutta method. In contrast to this, we use the second-order accurate Lie group generalized- α method proposed by Brüls et al. [Mech. Mach. Theory, vol. 48, 2012] for the time integration of the equations of motion and the kinematic reconstruction equation. To avoid drift in the holonomic constraints due to index-2 formulation, we use the stabilized index-2 generalized- α DAE integrator, which satisfies the holonomic constraints at position level and the corresponding hidden constraints at the velocity level at each time step [Arnold et al., CISM, vol. 565, 2016]. As configuration space

we choose the special Euclidean group $SE(3)$. The presented index-2 formulation is tested using a set of numerical tests for the benchmark problem of a rotating heavy top. We test the index-2 formulation both for the velocity projection along the side faces of a hexahedron and for the velocity projection along the side edges of a tetrahedron. Furthermore, we compare the numerical results of the formulation presented in this paper with an index-3 formulation and conventional rigid body coordinates.

On mechanical DAE systems within the framework of optimal control

Simeon Schneider (*Karlsruher Institute of Technology (KIT), Germany*)

17:10

Peter Betsch (*Karlsruher Institute of Technology (KIT), Germany*)

In mechanical optimal control problems, the constraints of the cost functional to be minimized correspond to the equations of motion of the underlying mechanical system. If generalized (or minimal) coordinates are used for the description of the mechanical system, Pontryagin's maximum principle results in the well-known necessary optimality conditions. However, for complex mechanical systems minimal coordinates are often difficult to find, so redundant coordinates are preferred. Thus the state equations of the optimal control problem assume the form of differential-algebraic equations (DAEs) governing the motion of the underlying mechanical system. In their original form the DAEs have differentiation index three. Alternatively, GGL-type index reduction can be applied to yield DAEs with index 2 [1]. The corresponding optimality conditions have been derived in [3], see also [1]. Alternative solution procedures rely on the so-called adjoint method [2], the indirect and the direct approach [1].

In the talk we will present different approaches to embed the underlying mechanical DAE system into the optimal control problem. The numerical performance of the alternative methods will be compared in the context of a representative model problem.

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Utilizing general relations of balance for the improvement of discrete mechanics time integration schemes: application to the double pendulum

Evgenii Oborin (*Johannes Kepler University Linz, Austria*)

17:30

Hans Irschik (*Johannes Kepler University Linz, Austria*)

Discrete mechanics time integration schemes appeared in the literature on dynamics of mechanical systems around 1970, see [1] for some elegant explicit time-integration discrete algorithms. The hypothesis followed and substantiated in the present contribution is that considerable improvements of such schemes can be achieved when they are substituted (as an initial guess) into the time-integral form of the balance relations, into the so-called general forms of the balance relations, [2]. In contrast to their differential counterparts, to which numerical time-integration schemes usually do refer, the integral forms obey less continuity requirements, and they may be considered as being more fundamental also from a physics viewpoint, [3]. Repeated substitution into the general balance relations leads to further improved explicit integration schemes. Utilizing the benefits of symbolic computer algebra codes, it is thus possible to establish time-stepping procedures in a straightforward manner.

Our hypothesis has been already successfully checked studying the plane motion (linear and nonlinear) of a mathematical pendulum, [4]. It has been shown that highly accurate explicit

algorithms can be achieved, which can well compete with higher-order implicit numerical integration schemes, and which yield accurate results also in case of long observation periods.

In [4] the general relation of balance of angular momentum has been utilized in the context of the mathematical pendulum. It is the scope of the present contribution to study the two-body problem of the double pendulum, involving also general balance of linear momentum, as well as the Lagrange equations, see [5]. Our present two-body study is intended as a first step in developing novel multi-body formalisms.

Literature

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Variational formulation and discretization of multi-body systems with fluid-structure interaction at low Reynolds number

Dominik Kern (*TU Chemnitz, Germany*)

17:50

Michael Gross (*TU Chemnitz, Germany*)

Although the advantages of structure-preserving time integration methods are well known, they are limited to components fitting into their framework. Common components in machines and mechanisms, which persistently defend against a variational formulation, are hydrodynamically lubricated contacts. Since there exists no variational principle for the Navier-Stokes Equations in general, only certain approximations, either for very high or very low Reynolds number, can be formulated as stationarity condition of certain functionals. In thin fluid films, such as lubrication films, typically the viscous terms dominate the inertial terms ($Re \ll 1$). This motivates the modeling of the fluid film between lubricated components as incompressible fluid, which is governed by Stokes Equations. The corresponding variational principle of the fluid dynamics, minimum of entropy production, is combined with Hamilton's Principle for multi-body systems. Velocity and pressure field in the fluid are spatially discretized by global approximations, which comply to the continuity equation and certain requirements for solutions of Stokes Equations. The remaining time discretization for the complete system, rigid or elastic bodies and fluid, follows the methodology of variational integrators. As long as the conditions for Stokes Equations are fulfilled, the obtained spatial resolution can be refined to arbitrary precision by increasing number of spatial approximation functions. Similarly, the error in time is controlled by order and stepsize of the approximation in time. As example serves a rotor in hydrodynamically lubricated sleeve bearings. The results for stationary and transient simulations of this rotor obtained with the proposed discretization scheme are compared to the popular Sommerfeld Solutions for the bearing forces in combination with a generic Runge-Kutta ode-solver.

S01.03 | Multi-body dynamics

Date: February 21, 2019

08:30-10:30

Room: HS 16

Consistent Euler-Lagrange approach for particulate flow modelling with arbitrary particle size/mesh resolution ratio

Fabien Evrard (*Otto-von-Guericke-Universität Magdeburg, Germany*)

08:30

Berend van Wachem (*Otto-von-Guericke-Universität Magdeburg, Germany*)

Euler-Lagrange approaches are widely used for the numerical modelling of complex particulate flows owing to their relatively low computational cost and the straightforward modelling of particle-particle interactions. Since relying on an assumption of separation of scales between the general features of the flow, which are resolved on the Eulerian fluid mesh, and those at the scale of the Lagrangian particles, which are modelled based on simplified theoretical/empirical models, Euler-Lagrange methods typically require the tracked particles to be much smaller than the cells forming the mesh on which the flow equations are solved. For cases that present high refinement requirements, for instance due to the presence of boundary layers or complex geometry features, this can drastically limit the size of the particles that can be accurately tracked within the flow. In this contribution, we propose an Euler-Lagrange approach that is free of such restrictions. It relies upon the filtering of the instantaneous flow equations with a particle marker function; a process in which a length-scale is chosen. This decouples the size of the particles with the specific length of the discretised mesh cells in calculating the volume fraction. This filtering is also applied to the fluid-particle momentum coupling terms, which provides a solid framework for spreading these source terms. Throughout the application of the proposed method to a number of test-cases, we show that the filtering strategy allows for the consistent tracking of Lagrangian particles regardless of their size relative to the Eulerian mesh. The method is then applied to large-scale particulate flows, namely: a turbulent channel flow and a fluidised bed, and the impact of the proposed filtering on the statistics of the flow is investigated.

An IGA-based three dimensional Cosserat rod for multibody dynamics

Simone Benatti (*Università di Parma, Italy*)

08:50

Alessandro Tasora (*Università di Parma, Italy*)

Dario Mangoni (*Università di Parma, Italy*)

We present a Cosserat beam model based on Isogeometric Approach (IGA). This approach uses splines (B-Splines or NURBS) in order to parametrize positions and orientations of the beam line of mass centroids leading to several advantages, such as the possibility of managing large non-linearities, and consequently large deformations. Furthermore using splines allows for direct import of CAD-created geometries thus representing shapes as accurately as possible and avoiding the computational cost of mesh discretization. The beam centerline positions are mapped to a spline in R^3 while orientation are parametrized in terms of unit quaternions by a 4-dimensional spline. The Cosserat beams takes into account shear deformation, thus this formulation is valid for thick beams. The beam model was implemented in the multibody dynamics engine Project Chrono.

Nodal-displacement-based derivation of the floating frame of reference formulation: avoiding inertia shape integrals

Andreas Zwölfer (*University of Innsbruck, Austria*)

09:10

Johannes Gerstmayr (*University of Innsbruck, Austria*)

An increasing focus on the optimization of products to higher levels of reliability and efficiency in combination with the growing complexity of our technology dominated world pushes industry away from physical towards virtual prototyping. Which is why, advanced engineering simulation tools have become indispensable to master today's challenges.

The well-established floating frame of reference formulation (FFRF) is the most widely used method to simulate flexible multibody systems relevant for industrial applications. The FFRF is suitable for problems characterized by large reference motions, i.e. rigid body translations and rotations, but small deformations, which is the case for a wide range of engineering devices. However, conventional implementations of the FFRF would require computationally expensive evaluations of inertia shape integrals during simulation; these volume integrals depend not only on the degrees of freedom, but also on the finite element (FE) shape functions. Hence, conventional FFRF implementations depend on the underlying FE code, where the continuous flexible bodies were discretized. These problems originate from the circuitous continuum-mechanics-based derivation of the FFRF reported in the literature and make conventional FFRF implementations laborious.

The current contribution entirely avoids the evaluation of the aforementioned shape integrals. The novelty of this approach lies in the nodal-displacement-based derivation of the FFRF equations of motion (EOM). The derivation starts in the already (spatially) semi-discretized domain, where the nodal displacements are split into translational, rotational and flexible parts, and the kinetic and potential energy are written in terms of the appropriate nodal displacements, the linear FE mass and stiffness matrices and the nodal force vector. The EOM are then derived with a Lagrangian approach for a general mechanical system and simplified by making use of the inherent properties of the arising matrices and vectors.

Besides the simple and concise derivation in the proposed approach, the standard linear FE system matrices need to be extracted only once during preprocessing and evaluations of inertia shape integrals are not required; instead, simple (sparse) matrix-vector multiplications, with the linear FE mass matrix involved, are performed. Which is why, this approach is fully decoupled from any FE package, requires just a few lines of code and holds, therefore, potential for the implementation on embedded systems required for real-time applications.

Finally, the new implementation is tested and illustrated by a representative example.

Model order reduction of structures with fractional viscoelastic coupling

Arne Leenders (*Leibniz University Hannover, Germany*)

09:30

Michael Burgwitz (*Leibniz University Hannover, Germany*)

Matthias Wangenheim (*Leibniz University Hannover, Germany*)

Elastomers exhibit viscoelastic behaviour, i.e. they have both, elastic and viscous properties. Consequently, deformations of such materials show partially dissipative and time-dependent behaviour. We propose to transform an elastomer component's mass and stiffness matrices derived from commercial FE software into a multi-body system (mbs), following the approach described by Ewins in "Modal Testing" [1]. Our final mbs then consists of point masses and coupling springs as well as fractional viscoelastic dampers which we use to model frequency and temperature dependent material properties of the rubber component. In particular we are interested in simulating transient deformations of elastomer components, e.g. the impact of a tire tread

block into the road surface once every revolution of the tire. The challenge and novelty in our approach is the implementation of different methods of model order reduction in spite of the nonlinear characteristics of the fractional dampers: We will show how we were able to reduce the model order to decrease computational effort successfully while the accuracy of the results is ensured. We will present simulation results on the example of a siped winter tire tread block performing transient movements.

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A new approach for the simulation of flexible multibody systems and its relation to existing ones

Robert Winkler (*Fachhochschule Kärnten, Austria*)

09:50

Johannes Gerstmayr (*Universität Innsbruck, Austria*)

Most simulation techniques for flexible multibody systems rely on the assumption that the motion of each body can be decomposed into the motion of a rigid body frame and a small flexible motion relatively to this frame. The model order can be reduced by approximating the flexible motion by a linear combination of a (usually small) number n of flexible modes. In the floating frame of reference formulation (FFRF), the degrees of freedom (DOFs) of each body consist of the rigid body coordinates and n flexible mode amplitudes. In contrast, the absolute coordinate formulation (ACF) applies coordinates relatively to an inertial frame. To account for the assumed characteristics of the overall motion, the applied strain measure is co-rotationally linearized leading to a co-rotational stiffness and a constant mass matrix. To enable a model order reduction, the original flexible modes have to be transformed to apply at the inertial frame, which gives rise to a total number of $12+9n$ generalized modes, including the rigid body modes (generalized component modes synthesis, GCMS). The FFRF can be recovered by eliminating the extra DOFs of the GCMS formulation via appropriate constraint conditions related to the rigid body motion. This can be achieved via a projection onto the null-space of the constraint Jacobian. This approach reveals the freedom to apply the projection to the whole set of GCMS DOFs, to the 12 rigid body DOFs only, or to the $9n$ flexible DOFs only. Referring to the latter choice, a formulation is obtained which takes an intermediate position: The number of flexible coordinates equals the one of the FFRF but the rigid body coordinates are the ones of the GCMS such that the linear configuration space of rotation parameters is untouched. The new formulation is more or less as easy to be implemented as the GCMS method. As for the FFRF, the mass matrix is non-constant and a nonlinear force vector appears which couples rotational and flexible velocities. However, updating the mass matrix and the nonlinear force vector is cheap since it is basically achieved by rotating constant vectors. It is noted that the 12 rigid body DOFs have to be constrained. This gives rise to six Lagrange multipliers, such that the total number of unknowns equals $18+n$. The new method is assessed numerically analyzing an elastic pendulum undergoing a three-dimensional motion.

S01.04 | Multi-body dynamics

Date: February 21, 2019

14:00-16:00

Room: HS 16

A model-based strategy for safety assessment of a robot arm interacting with humans

Nemanja Kovincic (*Johannes Kepler University Linz, Austria*)

14:00

Andreas Müller (*Johannes Kepler University Linz, Austria*)

Hubert Gattringer (*Johannes Kepler University Linz, Austria*)

Impact and the resulting contact forces can be determined by dynamic simulation once a validated model for the robot and of the contact area of the human is available. Methods for the identification of relevant geometric and dynamic parameters of the robot model are well established. While the experimental validation of constitutive models for human body contact is still topic of ongoing research, which gave rise to the ISO/TS 15066 guidelines, adequate models are already available for computational simulation of human-robot contact scenarios. However, dynamical simulations cannot be applied to exhaustively explore and assess all possible contact scenarios with the robot workspace. In this paper, first the model used for impact simulation is described and simulation as well experimental results are reported for contact at a predefined location. It is then shown how this model can be used to anticipate the impact at other points where no experimental measurements are available. Secondly, an assessment measure is introduced that allows for anticipating impact forces without a dynamic simulation, which is based on the concept of reflected mass.

Kino-geometric modeling: insights into protein molecular mechanisms

Dominik Budday (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

14:20

Sigrid Leyendecker (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

Henry van den Bedem (*SLAC National Accelerator Laboratory, Stanford University, USA, University of California, San Francisco, USA*)

Proteins are dynamic macromolecules that perform an immense variety of biological functions on a broad range of spatio-temporal scales. Their conformational ensemble is a fundamental determinant of functionality in health and disease, and thus, its structural and dynamic characterization has been a major research focus over the last 50 years. While computational advances have increasingly enabled the computation of atomically detailed trajectories from Molecular Dynamics (MD) simulations, there remain considerable drawbacks when aiming for fast, yet elaborate insights into the molecular mechanisms of function.

Here, we explore the potential of kinematics and geometry based methods to study protein conformational dynamics. To this end, we lay out a robotics-inspired, kino-geometric model that efficiently captures small- and large-scale collective motions in the molecule, with dihedral angles as torsional degrees of freedom and non-covalent interactions such as hydrogen bonds and hydrophobics as constraints. Using geometric tools, we demonstrate insights into molecular mobility from instantaneous rigidity and flexibility analysis on selected example systems. Resulting motions from kinematically sampling along collective degrees of freedom show qualitative and quantitative agreement with motions from MD simulations. Coupled to sophisticated motion planning strategies, our approach is capable of providing structural ensemble representations

from sparse experimental data such as double electron-electron resonance (DEER) that remain difficult to interpret otherwise. Given the fraction of associated numerical effort compared to MD, our results establish kino-geometric protein modeling as an efficient alternative to obtain high-level insights into molecular mechanisms across scales. Setting up a computational pipeline for protein dynamics, these results may serve as proficient input to fine-tune analysis using more detailed, costly methods such as MD, with broad applications in protein engineering, drug design, and human health.

Optimal planning and control of a Segway model taking into account spatial obstacles

Christian Zauner (*Johannes Kepler University Linz, Austria*)

14:40

Hubert Gatringer (*Johannes Kepler University Linz, Austria*)

Andreas Müller (*Johannes Kepler University Linz, Austria*)

Matthias Jörgl (*Trotec GmbH, Austria*)

This contribution focuses on the optimal trajectory planning for a Segway model (inverted pendulum on two independently actuated wheels). Basis for this planning is the dynamical model for this under actuated, non-holonomic multibody system. Special focus is on the derivation of the ground reaction forces since they are very important for trajectories with high accelerations. For the stabilization as well as the trajectory control, a partial input/output linearization is performed, where the orientation of the robot w.r.t. the horizontal plane and the inclination angle of the pendulum are used as output. The remaining non-linear part is linearized about the upright equilibrium position and stabilized with an LQR controller. The trajectory optimization is based on the partially linearized system, where the output (orientation and inclination) is parameterized by B-Splines. The system is required to move through predefined points in the horizontal plane. For the optimization the control points of the B-Splines serve as optimization variables and the overall energy of the robot serves as cost functional. Maximum motor velocities, motor torques and the ground reaction forces are the constraints. The latter are crucial when planning trajectories where the robot must pass (swing) under vertical obstacles while not losing ground contact. These maneuvers are characterized by high horizontal accelerations in order to lower the head of the robot and bring it back to upright equilibrium. Simulations as well as experimental results are presented.

Inverse dynamics of an industrial robot using motion constraints

Thomas Lauß (*University of Applied Sciences Upper Austria, Austria*)

15:00

Karim Sherif (*University of Applied Sciences Upper Austria, Austria*)

Wolfgang Steiner (*University of Applied Sciences Upper Austria, Austria*)

In multibody dynamics, holonomic constraint equations exist because of mechanical joints or specified motion trajectories. In order to solve the dynamic equations of motion of the constrained multibody system, one can use a coordinate partitioning approach to eliminate dependent coordinates. However, an alternative approach is to use the Lagrange multiplier technique. A generalized constraint force vector associated with the system generalized coordinates has to be added in the equations of motion, which is computed by a multiplication of the constraint Jacobian times a Lagrange multiplier. At this point, it should be noted that the constraint force vector is in general not the vector of actual reaction forces at the joints.

In robotics, it is of particular interest to prescribe the motion of the tool center point and determining the drive torques in the joints. This leads to an optimal control problem, which is in general very expensive to solve. However, an alternative method is to apply a motion as a rheonomic constraint equation on the tool center point of the robot. We show that the resulting

generalized constraint force vector, which is acting on the body of the tool center point, can be converted into the required drive torques in the joints by the use of the principle of virtual work. From this solution, the equivalent desired drive torques can be computed. The advantage of the proposed method is that the solution can be obtained after one single forward simulation of the multibody system. Since the conversion into the drive torques is just a post-processing step.

Numerical calculations of transient states taking into the consideration the friction in joints of medical robot using the FEM

Grzegorz Ilewicz (*University of Bielsko-Biala, Poland, Lodz University of Technology, Poland*) 15:20

Andrzej Harlecki (*University of Bielsko-Biala, Poland*)

The numerical model of a serial chain medical robot was created by using the finite element method. The model enables the solution of the equation movement for a deformable RRRS configuration of a medical robot. This equation includes inertia, damping and resilience, as well as a forcing action. In addition, friction in joints has been added in order to include the anti-motion reactions, which are important in the study of dynamics of medical robots due to the fact that the friction is a worthy of attention reason for its deterioration. The model is solved iteratively in such a way that the deformations from previous iterations are included in the next ones. The model allows to test the transient dynamics. An optimization task has been formulated for the created model. The criteria for the vector function was mass and the displacement of the effector. Its optimum was found using the Pareto fronts and the MOGA genetic algorithm.

Time-optimal control of a vehicle on a race track using a Pacejka tire model

Philipp Eichmeir (*University of Applied Sciences Upper Austria, Austria, Vienna University of Technology, Austria*) 15:40

Stefan Oberpeilsteiner (*University of Applied Sciences Upper Austria, Austria*)

Thomas Lauß (*University of Applied Sciences Upper Austria, Austria*)

Wolfgang Steiner (*University of Applied Sciences Upper Austria, Austria*)

Time-optimal control of multibody systems deals with the problem of finding control inputs minimizing the final time and taking into account some state inequality constraints. This task leads to a two point boundary value problem, which is hard to solve and requires an initial guess close to the optimal solution.

In order to solve the time-optimal control problem we propose the adjoint gradient computation method as it is more robust than solving the underlying two point boundary value problem. Using the gradient information, a minimum of a cost function can be found by applying the method of steepest descent or, more performant, the BFGS-algorithm.

Let us now consider the control inputs for accelerating, braking and steering a vehicle such that the lap time is minimal. A cost function is introduced, which characterizes the final time and a penalty function is used to satisfy inequality constraints such as the boundaries of the track, the side slip angle of the vehicle as well as the limitation to the steering angle.

In order to specify the final time, a stop criterion is required to recognize the end of a simulation run. For that purpose we use a scalar equation which is satisfied, when the finish line of the race track is crossed. To formulate such a transversality condition, we apply a transformation from Cartesian to curvilinear coordinates, where the vehicle position is described by the road lane center line and a distance measured normal to the center line.

For the application of the proposed theory we investigate a vehicle with a Pacejka tire model. Two control inputs, one for accelerating and braking and one for steering, are introduced and used within the optimization.

S01.05 | Multi-body dynamics

Date: February 22, 2019

08:30-10:30

Room: HS 16

On the origin of passive rotation in rotational joints, and how to calculate it

Shucen Du (*Hamburg University of Technology, Germany*)

08:30

Josef Schlattmann (*Hamburg University of Technology, Germany*)

Stefan Schulz (*Hamburg University of Technology, Germany*)

Arthur Seibel (*Hamburg University of Technology, Germany*)

In a Gough-Stewart platform, the base platform is usually connected to the moveable platform by six identical chains consisting of passive rotational joints and linear actuators. Here, a passive rotation of the rotational joints may be harmful because it may cause additional length variations of the linear actuators, such as lead screws, besides the demanded lengths (or additional stresses in the lead screws if the rotation is obstructed). In order to incorporate this change in lengths into the kinematics, there is the necessity to analyze the origin of passive rotation and the equivalence relation of the input and output angles of the rotational joints.

Rotational joints, such as universal, Rzeppa, Tracta, or Thompson joints, transmit rotations. A passive rotation of these joints is caused by the rotation of the input shaft or, if the input shaft is fixed, the variation of orientation of the output shaft of the joint.

Passive rotation can be classified as inequivalent and equivalent. An inequivalent passive rotation leads to a difference in the rotation angle between the joint's input and output shaft, whereas an equivalent passive rotation does not. The origin of this inequivalence is that the intermediate component of the joint cannot provide equal rotation axes with respect to the input and output axes, for example, the intermediate cross shaft in a universal joint. In contrast, the equivalent passive rotation exists in constant-velocity joints, such as Rzeppa joints, where the intermediate component provides equal rotation axes referred to both the input and output axis and the angle transmission in such joints is one-to-one. In contrast to that, no passive rotation occurs if the corresponding joint does not contain an intermediate element, such as the spherical joint.

Therewith, we can conclude that the origin of passive rotation of rotational joints is the (physical or fictitious) intermediate component that provides a rotation driven by the input axis. If there is no explicit rotation axis of the intermediate component, there is no passive rotation, just as it is with spherical joints and joints with a revolute pair along the input or output shaft.

In this work, we explain the origin of passive rotation in rotational joints and provide a method to calculate it. This method allows checking whether a joint is a constant- or an inconstant-velocity joint. Furthermore, we apply our method to three examples: the universal joint, the Rzeppa joint, and the Tracta joint.

On different geometric approaches to the dynamics of finite-dimensional mechanical systems

Simon R. Eugster (*University of Stuttgart, Germany*)

08:50

Giuseppe Capobianco (*University of Stuttgart, Germany*)

Tom Winandy (*University of Stuttgart, Germany*)

The language of differential geometry allows a coordinate free representation of physical quantities. This led to the development of several geometric theories for the description of finite-dimensional mechanical systems. These approaches differ in the mathematical concepts they invoke and in the classes of mechanical systems they can describe. This talk aims to give an

overview on the following popular approaches. In the first, the motion of the mechanical system is considered as a curve on the system's (Riemannian) configuration manifold. It will be shown that this description is limited to scleronous mechanical systems with velocity-independent forces. In a second approach in which the motion is interpreted as integral curve of a vector field on the tangent (resp. cotangent) bundle of the configuration manifold more general forces can be applied. This approach relies on a symplectic structure of the underlying bundle and characterizes the vector field by a real-valued function known as Lagrangian (resp. Hamiltonian). Finally, rheonomous mechanical systems can be treated by replacing the configuration manifold with a 'generalized space-time', a so-called Galilean manifold.

Kinematics of finite-dimensional mechanical systems on Galilean manifolds

Tom Winandy (*University of Stuttgart, Germany*)

09:10

Simon R. Eugster (*University of Stuttgart, Germany*)

Giuseppe Capobianco (*University of Stuttgart, Germany*)

To describe rheonomous finite-dimensional mechanical systems a generalized space-time is introduced as a so-called Galilean manifold. This manifold generalizes the notion of a four-dimensional space-time one would use for the description of a particle moving in three-dimensional space. The Galilean manifold is endowed with a time structure that allows to measure time locally w.r.t. some reference time. The time structure induces a local splitting of the generalized space-time into time and space. Points of the generalized space-time are called events. The local splitting associates each event with one time and several position coordinates. The set of positions of simultaneous events form a submanifold that is endowed with a Riemannian metric. Therefore, the notion of distance is available for simultaneous events as it is required by experimental observation. The state space of the mechanical system is modeled as an affine subbundle of the tangent bundle to the Galilean manifold. Finally, the motion of a mechanical system is introduced as an integral curve of a (second-order) vector field on the state space.

Dynamics of finite-dimensional mechanical systems on Galilean manifolds

Giuseppe Capobianco (*University of Stuttgart, Germany*)

09:30

Tom Winandy (*University of Stuttgart, Germany*)

Simon R. Eugster (*University of Stuttgart, Germany*)

As presented in the talk 'Kinematics of finite-dimensional mechanical systems on Galilean manifolds', the state space of a rheonomous finite-dimensional mechanical system is defined as an affine subbundle of the tangent bundle to the Galilean manifold modeling the generalized space-time of the system. The second-order vector field on the state space that describes the system's motion can be associated with a differential two-form called the action form of the mechanical system. In this talk, we postulate the action form for rheonomous finite-dimensional mechanical systems as well as a generalization of the principle of virtual work as a fundamental principle of dynamics. We derive Lagrange's equations of the second kind and Hamilton's equations from two coordinate representations of this principle.

S02 | Biomechanics

Organiser: Markus Böhl (*Technische Universität Braunschweig, Germany*)
Alexander Ehret (*EMPA, ETH Zürich, Switzerland*)

S02.01 | Biomechanics

Date: February 19, 2019
Room: HS 01

08:30-10:30

Challenges and perspectives in brain tissue testing and modeling

Silvia Budday (*Friedrich-Alexander University Erlangen-Nürnberg, Germany*) 08:30
Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology - Trondheim, Norway*)
Paul Steinmann (*Friedrich-Alexander University Erlangen-Nürnberg, Germany, University of Glasgow, UK*)
Ellen Kuhl (*Stanford University, USA*)

Brain tissue is not only one of the most important but also the most complex and compliant tissue in the human body. While long underestimated, more and more evidence confirms that mechanics play a critical role for brain function and dysfunction. Therefore, computational simulations and patient-specific modeling based on the field equations of nonlinear continuum mechanics can provide important insights into the underlying mechanisms of brain injury and disease that go far beyond the possibilities of traditional diagnostics. Realistic predictions of mechanobiological processes in the brain require mechanical models capable of capturing the complex and unique characteristics of this ultrasoft, highly heterogeneous and adaptive tissue. In recent years, however, contradictory experimental results have retarded progress, which can in part be attributed to the fact that most mechanical testing setups had originally been established for much stiffer materials and reach their limits when it comes to brain tissue [1].

Here, we carefully assess the challenges associated with brain tissue testing and modeling. Through a profound review of previously published experimental data [1,2], complemented by new experimental, analytical and numerical analyses, we work out the most important characteristics of brain tissue behavior on different length and time scales. In this context, we also numerically study undesired artifacts, which might have resulted from ill-chosen experimental setups and should be avoided in the future. Based on our analysis, we propose application-specific modeling approaches, which are as complex as necessary but as simple as possible. The presented considerations will, on the one hand, facilitate well-designed future experiments and, on the other hand, help to choose the appropriate constitutive law for a specific application. Comprehensive mechanical models that capture the complex mechanics of nervous tissue and are based on reliable and comprehensive experimental data are key to perform predictive simulations useful to the biomedical and clinical communities covering a wide range of applications and pathologies - to estimate risk of injury, plan surgical procedures, or predict progression of disease.

References

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- [2] S. Budday, G. Sommer, J. Haybaeck, P. Steinmann, G.A. Holzapfel and E. Kuhl, Rheological characterization of human brain tissue. *Acta Biomater.*, 60:315-329, 2017.

The multiphysics of prion-like disease: spreading and atrophy in neurodegeneration

Amelie Schäfer (*Stanford University, United States of America*)

09:10

Lise Noel (*Stanford University, United States of America*)

Johannes Weickenmeier (*Stevens Institute of Technology, United States of America*)

Alain Goriely (*University of Oxford, United Kingdom*)

Ellen Kuhl (*Stanford University, United States of America*)

Neurodegeneration will undoubtedly become a major challenge in medicine and public health because of demographic changes worldwide. More than 45 million people are living with dementia today and this number is expected to triple by 2050. Recent studies have reinforced the hypothesis that the prion paradigm, the templated growth and spreading of misfolded proteins, could help explain the progression of a variety of neurodegenerative disorders. However, our current understanding of prion-like growth and spreading is rather empirical. Here we show that a physics-based reaction-diffusion model can explain the growth and spreading of misfolded protein in a variety of neurodegenerative disorders [1]. We combine the classical Fisher-Kolmogorov equation for population dynamics with anisotropic diffusion and simulate misfolding across a representative section of the brain and across the brain as a whole [2]. Our model correctly predicts amyloid-beta deposits and tau inclusions in Alzheimer's disease, alpha-synuclein inclusions in Parkinson's disease, and TDP-43 inclusions in amyotrophic lateral sclerosis. Our results suggest that misfolded proteins in various neurodegenerative disorders grow and spread according to a universal law that follows the basic physical principles of nonlinear reaction and anisotropic diffusion. A more quantitative understanding of the timeline of neurodegeneration could have important clinical implications, ranging from estimating the socioeconomic burden of neurodegeneration to designing clinical trials and pharmacological intervention.

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[2] Weickenmeier J, Jucker M, Goriely A, Kuhl E. A physics-based model explains the prion-like features of neurodegeneration in Alzheimer's disease, Parkinson's disease, and amyotrophic lateral sclerosis. *J Mech Phys Solids.* 2019; 124: 264-281.

Modeling disease-dependent elastic fiber degradation in aortic dissection

Malte Rolf-Pissarczyk (*Graz University of Technology, Austria*)

09:30

Kewei Li (*Graz University of Technology, Austria*)

Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology, Norway*)

An aortic dissection can be a life-threatening cardiovascular disease which is usually initiated by a tear in the intimal layer of the aortic wall. In most cases, it gradually propagates along the medial layer and creates a false lumen. Subsequently, it may lead to a complete rupture of the aortic wall followed by a fatal hemorrhage. It is agreed that the alteration of constituents in the aortic wall may be the initiation [1]. The degradation of elastic fibers and the resulting disorganization of the aortic wall structure is mentioned in this context frequently [1].

In the present study, on the basis of a continuum mechanics approach a constitutive model is presented to describe the disease-dependent degradation of elastic fibers in aortic dissection. It is of particular interest to examine the alteration of interlamellar elastic fibers, given the fact that they form bonds between the multiple layers of elastic lamellae, and thus have an important contribution to the composition of the aortic wall [1]. Ruptured interlamellar elastic fibers may

evoke due to the accumulation of pooled Glycosaminoglycans [1], and lead to a degraded material response especially concerning shear and tensile stresses in the radial direction.

The constitutive model assumes an additive split of the strain-energy function in three parts: groundmatrix, collagen fibers and elastic fibers. Subsequently, the parts are multiplied by the volume fraction of the specific constituent, respectively, so that the total volume fraction is equal to one. The groundmatrix is described by the isotropic neo-Hookean material model [2]. A discrete fiber dispersion approach with a von Mises distribution function is implemented for demonstrating the behavior of the collagen and elastic fibers, so that the collagen fiber distribution around a mean value can be described by a concentration parameter on the one hand [2], and the elastic fiber degradation in aortic dissection is modeled by the distribution function due a degradation parameter on the other hand. Finally, the constitutive model is implemented in the finite element analysis program FEAP and three representative numerical examples are chosen to demonstrate the performance with respect to aortic dissection.

References:

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[2] K. Li, R.W. Ogden and G.A. Holzapfel: A discrete fibre dispersion method for excluding fibres under compression in the modelling of fibrous tissue. *J R Soc Interface.* 2018;15(138).

A computational model for soft biological tissues considering the influence of injury on growth and remodelling

Meike Gierig (*Leibniz Universitaet Hannover, Germany*)

09:50

Michele Marino (*Leibniz Universitaet Hannover, Germany*)

Peter Wriggers (*Leibniz Universitaet Hannover, Germany*)

When soft biological tissues have physiological properties, deposition and degradation of tissues' constituents balance each other. In contrast, loading the tissue above its physiological limit causes injury. Injury activates a cascade of cell-cell interactions whereof a pathological imbalance of the arrangement and content of constituents result. Those growth and remodelling (G&R) processes affect the functionality of the tissue and the mechanical properties of the biological structure change. Such a case occurs, e.g., due to stent deployment in atherosclerotic arteries.

In this work, an approach for the computational modelling of soft biological tissues is proposed. Herein, the theories of plasticity and homogenized constrained mixtures are combined to account for the impact of injury on G&R. In detail, an elastoplastic model [1] is used to simulate the permanent stretch in tissue constituents due to the unphysiological loading. The deformation gradient is decomposed into an elastic and a plastic part and a Helmholtz free energy is formulated to incorporate the anisotropic mechanical response of the tissue. The evolution of plastic deformation is interpreted as an indicator of injury. Following the injury, G&R is activated. This is modelled considering a further multiplicative split of the inelastic part of the deformation gradient and following the homogenized constrained mixture theory. Here, the G&R inelastic deformation captures the gross (time-averaged) effects related to stress-free changes induced by mass variations of each constituent [2].

Following the slow-growth assumption, the time-scales of growth and elastoplastic deformations can be clearly separated. As a consequence, the plastic deformation and G&R are implemented in a staggered way. The model is evaluated simulating the expansion of an artery segment. The results show that injury has a significant impact on the G&R behaviour and motivate the extension towards a chemo-mechano-biological material model [3].

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Modeling of the corrosion-fatigue behaviour of biodegradable magnesium alloys

Songyun Ma (*RWTH Aachen University, Germany*)

10:10

Bernd Markert (*RWTH Aachen University, Germany*)

Biodegradable magnesium alloys are regarded as promising biomaterials of the next-generation orthopaedic implants. Biodegradable orthopaedic fixation systems potentially avoid a second surgery for implant removal, which alleviates pain and disability for patients, and thereby reduces socioeconomic burdens of health care systems. Despite these advantages, a number of fundamental problems have to be solved for promoting the development and breakthrough of the biodegradable magnesium implants. One major challenge is to tailor the biodegradable implants with adequate corrosion rate, sufficient mechanical strength and minimized mass, which require a deep understanding of the corrosion behaviour and a quantitative description and the degradation of mechanical integrity under physiological loadings.

In the present work, a nonlocal corrosion-fatigue damage model is proposed to describe the corrosion-fatigue damage behaviour based on the experimental results from corrosion-fatigue tests in simulated body fluid. The corrosion and fatigue damage variables are defined to represent the mass loss of material and the fatigue crack. Furthermore, a nonlinear accumulation law is used to describe the interaction between pitting corrosions and fatigue crack growth. The proposed nonlocal damage model is implemented within the framework of finite element method. An efficient numerical algorithm of the integral-type nonlocal damage model is developed for reducing the computational cost of simulations with a large number of cycles. The simulation results show that the proposed damage model provides a reasonable prediction of the corrosion-fatigue behaviour of biodegradable magnesium alloys under cyclic loadings in physiological environments.

S02.02 | Biomechanics

Date: February 19, 2019

16:30-18:30

Room: HS 01

Computational modeling of adhesive contact between a virus and a cell during receptor driven endocytosis

Tillmann Wiegold (*TU Dortmund University, Germany*)

16:30

Sandra Klinge (*TU Dortmund University, Germany*)

Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology (NTNU), Norway*)

Robert P. Gilbert (*University of Delaware, USA*)

The present contribution deals with the viral entry into a cell dictated by the change of the receptor density. While the receptors of the virus are considered to be fixed on its surface, the ones of the cell are mobile within its membrane. Upon contact, a locally increased receptor density of the cell is required, which causes them to diffuse towards the virus. In the contact (adhesion) zone the membrane inflicts and forms an envelope around the virus. The vesicle

created in this process imports its cargo into the cell. The described problem is simulated based on the assumption that the differential equation typical of the heat transport is suitable to describe the diffusion of receptors. Furthermore, two boundary conditions are proposed. The first condition deals with the balance of fluxes on the front of the adhesion zone, where the velocity is supposed to be proportional to the gradient of the chemical potential. The second condition represents the energy balance equation with contributions due to the binding of receptors, the free energy of the membrane, its curvature and the kinetic energy due to the motion of the front. The corresponding moving boundary problem is well posed and can be solved by applying a direct numerical method. This contribution applies the finite difference method to this end. The selected numerical example shows the change of receptor density over the membrane as well as the motion of the front of the adhesion zone. Special attention is paid to the mobility of the receptors.

Continuum-mechanical modelling of apoptosis

Patrick Schroeder (*University of Stuttgart, Germany*)

16:50

Arndt Wagner (*University of Stuttgart, Germany*)

Daniela Stoehr (*University of Stuttgart, Germany*)

Markus Rehm (*University of Stuttgart, Germany*)

Wolfgang Ehlers (*University of Stuttgart, Germany*)

In cancer cells, apoptosis, a mode of cell death, can be induced by administration of drugs such as TRAIL. This reagent shifts the cell internal inhibition and activation reactions towards the activation of caspases, triggering the cell death. The description of apoptosis on the macroscopic scale including the tissue, where the cancer cells are situated in, as well as the surrounding fluids, leads to a rather complex model.

Therefore, this contribution compares two continuum-mechanical models including either a simplified description of apoptosis or a model including an apoptotic pathway using an ordinary differential equation system. Further on, these two models are compared to cancer-cell-survival experiments in the presence of different TRAIL concentrations. In particular, the general model is specified for lung-cancer metastases located in brain tissue. Thus, the hyperelastic solid is characterised by brain cells and the metastases. The solid is saturated with two immiscible pore liquids, namely the blood and the interstitial fluid. The latter is a real mixture of the energy-supplying nutrients, the infused drug and the solvent. The essential variation in the models are related to the calculation of the mass-production term of apoptosis. The simplified model version inheres on a constitutive logarithmic proliferation function for the apoptotic mass-production term, whereas the general approach includes a system of locally solved ordinary differential equations. In both models, adapted mass balances and the overall momentum balance are solved for the solid displacement, the liquid pressures and the concentrations. Numerically, the finite-element code PANDAS is used, where Taylor-Hood elements are applied for the spacial discretisation and an Euler time-integration scheme discretising the time.

Finally, both models are compared to apoptosis experiments measuring the survival rate of lung-cancer cells in dependency of the TRAIL concentration.

Modeling the vesicle motion through the cytoplasm

Daniel Christopher Haspinger (*Graz University of Technology, Austria*)

17:10

Sandra Klinge (*TU Dortmund University, Germany*)

Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology (NTNU), Norway*)

One of the most characteristic property of eukaryotic cells is the high level of organization of their internal transport processes, especially the vesicle-mediated cell transport. Thereby, the

cargo gets packed into vesicles, which form out of the donor membrane. Subsequently, vesicles move through the cytoplasm, i.e. through the cytosol and along a microtubule by means of motor proteins (kinesin and dynein), until they find their correct destination and fuse with organelles or the plasma and finally deliver their cargo. The precise manner of the routing process can be illustrated by numerous examples such as the release of neurotransmitters into the presynaptic region of a nerve cell or the export of insulin to the cell surface. The interior of a cell is a complex composite material which consists of water, structural scaffoldings (network of actin filaments, microtubules, intermediate filaments, etc.), organelles, and various biomolecular solutes. All of these serve as obstacles that impede the motion of vesicles within the cytosol. This motion is commonly simulated as diffusion within a mixture of two materials: the solvent having a certain diffusion coefficient, and the obstacles with the diffusion coefficient zero. However, especially this highly heterogenous micro-structure of eukaryotic cells on many different scales and the high contrast in physical properties are the key features for their behavior and functions. The consideration of all this detailed information is numerically extremely expensive while a naive disregard of relevant microscopic information leads to questionable results, even on macroscopic scales of interest. Therefore, for modeling the transport, the application of the diffusion model together with homogenization strategies appears to be a suitable approach because of the high complexity of the cytoskeleton.

The main objective of this study is to couple the results obtained from biomedical investigations and the mechano-mathematical model with highly efficient engineering software packages to simulate dynamic processes in eukaryotic cells, especially the vesicle transport. Disruption of the vesicle transport is thought to contribute to several severe diseases, such as amyotrophic lateral sclerosis (ALS), Alzheimer's disease, diabetes, etc. Hence, if we are able to fully understand and model the vesicle motion in health, efficient and validated computer models may help us to better understand the initiation and progress of diseases, where vesicle trafficking defects are included or driving forces, respectively.

Modelling cell motility as an active liquid crystal film with evolving free boundary

Georgy Kitavtsev (*University of Oxford, United Kingdom*)

17:30

Andreas Münch (*University of Oxford, United Kingdom*)

Barbara Wagner (*Weierstrass Institute for Applied Analysis and Stochastics, Germany*)

In this talk, we model the complex problem of description of cell motility as the Adenosinetriphosphate (ATP) driven motion of a thin film of actin filament network. Basing on existing approaches for modelling the actin filaments as an active liquid crystal bio-material we employ the Beris-Edwards theory that uses a tensorial order parameter and includes additionally active contributions to the stress tensor. The small aspect ratio of the film geometry allows for an asymptotic approximation of the free-boundary problem in the limit of weak elasticity of the network and strong active terms. The new thin film model captures the defect dynamics in the bulk as well as wall defects and thus presents a significant extension of previous models based on the Leslie-Erickson-Parodi theory. Analytic expressions are derived for special classes of stationary solutions.

On the comparison of mechanical properties of milk fouling and whey protein isolate fouling using of indentation tests

Jintian Liu (*Technische Universität Braunschweig, Germany*)

17:50

Hanna Wiese (*Technische Universität Braunschweig, Germany*)

Wolfgang Augustin (*Technische Universität Braunschweig, Germany*)

Stephan Scholl (*Technische Universität Braunschweig, Germany*)

Markus Böl (*Technische Universität Braunschweig, Germany*)

Due to the increasing standards for health and hygiene, cleaning in place (CIP) is widely applied as an integral part of the automated plant to wash away the undesired fouling from the heating surface. It can be achieved by a combination of thermal energy, mechanical flow, and chemical dissolution. The cleaning agent reacts with the fouling at a suitable temperature and reduces its cohesive and adhesive strength, which is then removed by turbulent flow, i.e. by mechanical forces. In view of the required water and cleaning agent costs, there is a large interest to optimise the CIP process by identifying limiting steps and adjusting the key parameters to improve the cleaning performance. For this, studies have so far tended to focus on the impact of chemical conditions, in which whey protein as the key component of the heat-induced fouling, has been used as a surrogate to mimic the formation of fouling and chemical cleaning processes. In most of these studies, cleaning efficiency was indicated by measuring the amount of the remaining fouling deposit over cleaning time. In addition, there is a shortage of further study in the aspect of mechanical properties of milk fouling deposit, which makes it hard to paint a clear picture of the mechanical removal of the milk fouling. To develop a deeper understanding of the mechanical properties of fouling, deposits in plate heat exchangers generated with raw milk and whey protein isolate (WPI) solution were investigated by carrying out cyclic indentation and relaxation experiments. It was intended to determine the mechanical characteristics of both kinds of deposits and to examine the comparability with each other. The results of both soils showed increasing nonlinear force responses with the strain. For milk fouling, an association between the force response and the fouling thickness was found. All the measured data can be categorized into three groups according to the thickness. The mean value of the forces approached on thicker deposits is larger than that of thinner ones. To characterise the loading behaviour of milk fouling, inverse finite element method coupled with Ogden material model was applied. Furthermore, for whey protein fouling, a relationship between the mechanical behaviours and the content of whey protein of the corresponding processing fluid was found and a suitable value of the content was suggested, which resulted in a relative good comparability with the milk fouling.

S02.03 | Biomechanics

Date: February 20, 2019

08:30-09:30

Room: HS 01

Numerical simulation of viscoelastic effects during bubble-collapse driven tissue-penetration

Naeimeh Hosseini (*Technical University of Munich, Germany*)

08:30

Stefan Adami (*Technical University of Munich, Germany*)

Nikolaus A. Adams (*Technical University of Munich, Germany*)

It is essential to understand the mechanism by which shock waves affect biological tissues in clinical application, such as extra-corporeal lithotripsy. Therefore a multi-material compressible solid-fluid solver is developed in a two-dimensional Eulerian framework. The method uses a

level-set function for tracking the sharp interface between individual materials, and treats each material independently using its own constitutive law.

Most of the available numerical investigations done previously use a fluidic material model to simulate the effect of shock waves in soft-tissues. However, this approach is only reasonable in early stages where elasticity and plasticity effects in the material are not dominating. Therefore, to study late stage effects, a more realistic material model for the tissue-surrogate phase is required.

In the current study, the viscoelastic material is modeled via a generalized equation of states (EoS) including the deformation. The evolution of the deformation gradient tensor is governed by an additional advection equation. As can be shown analytically the resulting system of equation is purely hyperbolic and can thus be solved within the original framework of the flow solver. We employed a weighted essentially non-oscillatory (WENO) scheme to achieve high-order accuracy, and a second-order Runge-Kutta method for the time-stepping scheme. Moreover the multi-resolution technique is used.

To model the interaction between solid and fluid material a locally non-conservative scheme is implemented based on the method of Gorsse et al. (*J. Comp. Phys.* 272 (2014) 772-798), while a conservative interface interaction scheme is used at fluid-fluid interface. (*J. Comp. Phys.* 219 (2006) 553-578). The former mentioned method for modeling the solid phase is adapted to be able to model the soft-tissues more accurately considering the viscoelastic effect in the new material model. The coupling at the solid-fluid material contact is determined by considering the specific boundary condition each material poses at the interface, and solving the resulting Riemann problem to determine the numerical fluxes.

In this work, the shock-induced bubble collapse near a viscoelastic material is studied, which represents a surrogate model for investigating the phenomenon occurring in soft-tissues subject to shock waves. The scheme is validated using one-dimensional initial value problems with exact solutions, and two-dimensional problems from the literature. In comparison to previous studies, in which a fluidic model is considered for the tissue phase, we expect more accurate results illustrating the penetration in soft-tissues due the effect of the bubble collapse.

A study on nanoparticle transport in a micro blood vessel

Mahrokh Bavandi (*University of Kassel, Germany*)

08:50

Olaf Wünsch (*University of Kassel, Germany*)

Magnetic drug targeting is a new technique to deliver drugs to a specific location of patient's body [1]. The aim is to reduce the amount of drugs and unnecessary side effect on healthy tissues, but the efficiency of the method depends on physical and physiological conditions e.g. the vessel size.

Blood is a suspension of blood cells in plasma. It is known that in micro-vessel flows there are less blood cells close to the walls, known as the Fahraeus-Lindqvist effect. The present study focuses on the investigation of the influence of this phenomenon in a micro-channel on nanoparticle transport.

To describe the multi component behaviour of blood, an Euler-Euler approach is used as proposed in [2]. Plasma is considered as a Newtonian phase and red blood cells as non-Newtonian. An interaction is modelled by lift and drag forces. A convection-diffusion equation is applied to model the concentration of nanoparticles. Studies are performed for different Reynolds numbers for a simple micro-channel configuration. For simulation, the approaches are implemented in OpenFOAM.

[1] Bulte, Jeff WM, et al.: "Design and applications of nanoparticles in biomedical imaging". Basel, Switzerland: Springer International Publishing, 2017.

[2] Wu, Wei-Tao, et al.: "Study of blood flow in several benchmark micro-channels using a two-fluid approach." *International journal of engineering science* 95, 49-59 (2015).

Validation study of computational fluid dynamics models of hemodynamics in the human aorta

Jana Fuchsberger (*Karl-Franzens-University Graz, Austria*)

09:10

Elias Karabelas (*Karl-Franzens-University Graz, Austria*)

Philipp Aigner (*Medical University of Vienna, Austria*)

Heinrich Schima (*Medical University of Vienna, Austria*)

Gundolf Haase (*Karl-Franzens-University Graz, Austria*)

Gernot Plank (*Medical University of Graz, Austria*)

Background and Introduction: Computational fluid dynamics (CFD) models of blood flow in the left ventricle and aorta show high promise as a tool for analyzing the mechanistic links between myocardial deformation and flow patterns as these are able to provide additional biomarkers not measurable at a higher spatio-temporal resolution than feasible with currently used clinical imaging modalities. However, before CFD tools can be applied for routine clinical evaluations the limits of their validity and accuracy of simulations must be characterized. In this vein we report on conducting a rigorous validation study where we attempt to compare simulated hemodynamics in a mock model of the human aorta with experimental bi-plane particle image velocimetry (PIV) data.

Methods: Within the cardiac modeling framework CARP (Cardiac Arrhythmia Research Package) we implemented a finite element CFD solver based on the residual-based variational multiscale (RBVMS) discretization of the incompressible Navier-Stokes equations. Using the PIV measurements 2D inflow boundary profiles were recovered by polar interpolation of velocity data sampled from the two orthogonal PIV imaging planes. Subsequently the comparison of simulated and experimental data was carried out using the following techniques. On the one hand methods for vortex identification based on the velocity gradient tensor were used to compare vortex structures in turbulent areas of the fluid domain. On the other hand dynamically distinct regions were compared using Lagrangian coherent structures, an analysis of time dependent dynamical systems using finite-time Lyapunov exponents.

Results: The compared flow characteristics agree well between simulation and PIV data, with deviations in the range of the overall measurement uncertainty.

Conclusions: CFD simulation results compare favorably with experimental PIV data suggesting that our CFD analysis tools are representative of blood flow in the human aorta.

S02.04 | Biomechanics

Date: February 20, 2019

14:00-16:00

Room: HS 01

Experimental micro- and nanomechanics of collagen rich-tissues and individual collagen fibrils

Philipp J. Thurner (*TU Wien, Austria*)

14:00

Orestis G. Andriotis (*TU Wien, Austria*)

Sylvia Desissaire (*TU Wien, Austria*)

Mark G. Jones (*University of Southampton, UK*)

Donna E. Davies (*University of Southampton, UK*)

All tissues providing passive mechanical function are rich in collagens, which are thought to provide stiffness and toughness, whereas resilience is thought to be provided by elastin. Macroscopically, relationships between tissue-structure, composition and mechanical function have

been explored but comparatively little has been done in this context on the micro- and nanometer length scale. Yet, perhaps the most important basic structural building block of collagen-rich tissues can be found between these scales: the collagen fibril. Fibrils are rope-like with diameters in the range of tens to hundreds of nanometers and they have extremely high aspect ratios with lengths reaching up to tens of millimeters. The capacity to measure mechanical properties at these levels is increasing continuously due to the development of approaches based on atomic force microscopy or MEMS devices. So far, investigations have shown interesting insights but a full and systematic view detailing structure-mechanical-function relationships for individual collagen fibrils and collagen-rich tissue micromechanics is still missing.

Insights into tissue mechanics at these levels are not only interesting from a basic science perspective, but are also important for understanding changes due to age and disease. That is, they may offer targets for diagnostics and treatment of pathologies. Furthermore, micro- and nanomechanics can be useful to elucidate mechanobiological effects as cells sense their environment at this level.

To elucidate this, examples will be presented demonstrating that tissue micromechanics and collagen fibril mechanics are dependent on the molecular structure of the tropocollagen molecule, chemical composition including chemical modifications (cross-links) as well as chemical environment, i.e. hydration. A specific focus is osmotic pressure and cross-linking. The effect of osmotic pressure has so far not been considered much on the level of individual collagen fibrils, but it exhibits significant influence on collagen mechanics. By employing poly-ethylene-glycol (PEG) as an osmotic pressure generating agent we found up to a six-fold increase in tensile stiffness of individual collagen fibrils. This elucidates the importance of hydration and noncovalent interactions for tissue mechanics. Classically, cross-linking of collagen is thought to be the major mechanism for tuning elasticity. We show that this effect is also present on the microscale. However, whether such cross-links have an effect on the tensile mechanics of individual collagen fibrils remains to be shown. It may well be that chemical cross-linking is more active in the extracellular space, linking fibrils together, rather than tuning mechanics of individual fibrils. Further research is required to clarify this.

Continuous versus discrete modeling of fiber dispersion in fibrous soft tissues

Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology (NTNU), Norway*) 14:40

Kewei Li (*Graz University of Technology, Austria*)

Ray W. Ogden (*University of Glasgow, UK*)

Selda Sherifova (*Graz University of Technology, Austria*)

Gerhard Sommer (*Graz University of Technology, Austria*)

Collagen fibers within fibrous soft tissues are responsible for their anisotropic mechanical behavior. It has recently been recognized that the dispersed orientation of these fibers has a significant effect on the mechanical response of the tissues, as reviewed in [1,2]. Modeling of the dispersed structure is important for the prediction of the stress and deformation characteristics in (patho)physiological tissues under various loading conditions.

This talk presents two approaches to the modeling of fiber dispersion, the continuous and the discrete approach, with the pros and cons critically discussed. The discrete fiber dispersion model, as proposed in [3], is based on a systematic method for discretizing a unit hemisphere into a finite number of elementary areas, such as spherical triangles. Over each elementary area, we define a representative fiber direction and a discrete fiber density. Then, the strain energy of all the fibers distributed over each elementary area is approximated based on the deformation of the representative fiber direction weighted by the corresponding discrete fiber density. A summation of fiber contributions over all elementary areas then yields the resultant fiber strain

energy. This treatment allows the exclusion of fibers under compression in a discrete manner by evaluating the tension-compression status of the representative fiber directions only.

The models are used in representative numerical examples to fit sets of experimental data that have been obtained from mechanical tests and fiber structural information from second-harmonic imaging. In particular, patches of healthy and diseased tissues are investigated.

References

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- [2] G.A. Holzapfel, R.W. Ogden and S. Sherifova: On fibre dispersion modelling of soft biological tissues: a review. *Proc. R. Soc. Lond. A*, submitted.
- [3] K. Li, R.W. Ogden and G.A. Holzapfel: A discrete fiber dispersion method for excluding fibers under compression in the modeling of fibrous tissues. *J. R. Soc. Interface*, 15: 20170766, 2018.

A microstructural model of crosslink interaction between collagen fibrils in the human cornea

Marcello Vasta (*University of Chieti Pescara, Italy*)

15:00

Alessio Gizzi (*Campus Biomedico, Rome, Italy*)

Anna Pandolfi (*Politecnico di Milano, Milan, Italy*)

Keratoconus is a progressive non-inflammatory disorder of the cornea that alters dramatically the shape of the lens from sphere to conus through a localized thinning. From the macroscopic point of view, in contrast to healthy corneas, keratoconic corneas present a conical curvature, which induces ruptures and anomalous deposition of chemical species. Microscopically, keratoconus is associated to degenerative changes in the organization of the reinforcing collagen fibrils of the cornea, which are embedded into an isotropic matrix of elastin and proteoglycans [1].

The particular microstructure of the collagen suggests that the macroscopic changes of the geometry in the keratoconus pathology are related to the weakening of the bonds (crosslink) between the collagen fibrils. It is generally acknowledged that corneal fibrils, well distinguished in two orthogonally oriented sets, assume a complex yet smooth configuration to provide a general confinement to the intraocular pressure (IOP), to support the eyelid opening and closure and the action of the muscles that rotate the eyeball, and to accommodate the functional transition between cornea and sclera.

In a first attempt to develop a physically based model of keratoconus onset and progression, in this study we present a simplified model of the collagen microstructure of the human cornea. The model consists in a trusswork that describes the two sets of fibrils and the hypothesized crosslinks connecting the fibrils. Clearly the model does not pretend to deliver a quantitative estimate of the deformation and of the stress within a keratoconus cornea, but it tries to understand the function of the different components of the fibril network in the preservation of the quasi-spherical configuration of the cornea.

We analyze the mechanical response of the system according to the type of interlacing and on the stiffness of the bonds. Results show that the weakening of transversal bonds is associated to a marked increase of the deformability of the system. In particular, the deterioration of transversal bonds can justify the loss of stiffness of the stromal tissue resulting in localized thinning and bulging typically observed in keratoconus corneas.

References

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Key factors for soft tissue tensional homeostasis identified by discrete fiber network modeling and biaxial experiments

Jonas F. Eichinger (*Technical University of Munich, Germany, Hamburg University of Technology, Germany*)

15:20

Daniel Paukner (*Yale University, USA*)

Roland C. Aydin (*Helmholtz-Zentrum Geesthacht, Germany*)

Jay D. Humphrey (*Yale University, USA*)

Christian J. Cyron (*Hamburg University of Technology, Germany, Helmholtz-Zentrum Geesthacht, Germany*)

Soft biological tissue is composed of cells and the extracellular matrix, a network of diverse filamentous proteins. In these tissues, a mechanism exists that seeks to achieve or maintain a preferred level of stress, a physiological behavior called tensional homeostasis. Cells are able to actively sense and regulate the mechanical stress to ensure tissue integrity for example during tissue repair in response to disease or injury. To allow for this essential two-way feedback loop consisting of mechanosensation and mechanoregulation, cells are attached to the extracellular matrix via transmembrane linker proteins, so-called integrins. These are in turn connected to the actin cytoskeleton which enables the cells to actively apply forces to their surrounding matrix. This talk presents a novel computational framework for modeling cell-extracellular matrix interactions in three dimensions based on the finite element method. Matrix fibers are modeled individually using one-dimensional geometrically exact beam finite elements to account for their bending as well as extensional stiffness. Non-elastic remodeling of matrix fibers by the inherent cells is captured by a model for dynamic inter-fiber crosslinking considering force dependent unbinding. Cells are also discretized by finite elements and able to attach to predefined, discretization-independent binding sites on the matrix fibers. These links between cells and matrix follow a specific molecular clutch model and are endowed with the ability to contract. We prove that our framework is capable of reproducing results that were collected from experiments with cell seeded tissue equivalents performed within a custom built biaxial bioreactor. Initially stress-free collagen gels seeded with fibroblasts were uniaxially and biaxially loaded over several hours while collecting displacement and force data. We will show the influence of various factors like collagen concentration, cell density as well as type of boundary condition on soft tissue tensional homeostasis.

DNA beams: molecular-to-beam upscaling - theoretical foundations and application to DNA

Johannes Kalliauer (*TU Wien - Vienna University of Technology, Austria*)

15:40

Stefan Scheiner (*TU Wien - Vienna University of Technology, Austria*)

Gerhard Kahl (*TU Wien - Vienna University of Technology, Austria*)

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

Mechanical properties of DNA are of great biological interest, as duplication and expression are, as a rule, processes involving force-driven deformations.

Traditionally, DNA sequences are considered as cylindrical straight isotropic beams [1], but this to unrealistic ratios between torsional and bending stiffnesses [2].

The deformation characteristics of long biological macromolecules, such as DNA or collagen, can be lucidly described by the terms “bending”, “stretching”, “torsion” and “shearing”. These terms appear in a subset of continuum mechanics, called beam theory, while the standard numerical modelling procedure for macromolecules, which is molecular dynamics, does not allow for a direct introduction of these deformation characteristics in the principle of virtual power [3].

This deficit has motivated the theoretical development of a transition or upscaling procedure from molecular dynamics to beam theory, which is the focus of this contribution. It consists of two steps:

- (i) translation of potential energies into systems of equilibrated forces and moments, while formally representing interaction lines between atoms as rigid beams - this allows for energetically consistent introduction of the “method of sections”, the key concept of continuum mechanics;
- (ii) upscaling, through the principle of virtual power, the forces and moments arising from (i), to the scale where the macromolecule itself is considered as a beam structure.

As a first application, the above-described novel strategy is realised for a sequence of DNA base pairs, elucidating the source of the somehow paradox stretching-torsion coupling these molecules are known for.

References

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- [2] Christoph G. Baumann, Steven B. Smith, Victor A. Bloomfield, and Carlos Bustamante. Ionic effects on the elasticity of single DNA molecules. *Proceedings of the National Academy of Sciences*, 94(12):6185-6190, June 1997.
- [3] Chunyu Li and Tsu-Wei Chou. A structural mechanics approach for the analysis of carbon nanotubes. *International Journal of Solids and Structures*, 40(10):2487-2499, May 2003.

S02.05 | Biomechanics

Date: February 20, 2019

16:30-18:30

Room: HS 01

Computational study of ventricular fibrillation by considering a strongly coupled electromechanical rat heart model

David Holz (*University of Erlangen-Nuremberg, Germany*)

16:30

Minh Tuan Duong (*University of Erlangen-Nuremberg, Germany*)

Muhannad Alkassar (*University of Erlangen-Nuremberg, Germany*)

Sven Dittrich (*University of Erlangen-Nuremberg, Germany*)

Sigrid Leyendecker (*University of Erlangen-Nuremberg, Germany*)

The European Heart Network (EHN) published in the European Cardiocascular Disease Statistics 2017 a total number of 3.9 million deaths per year and proportionate to all death around 45%. Ventricular fibrillation itself is the most common cause of sudden death. We present a computational study about the source, evolution and termination of ventricular fibrillation by considering a strongly coupled electromechanical rat heart model on a tissue/ organ level (tissue heterogeneities). As a model of human cardiovascular disease, rats are widespread in today’s medical reseach due to the fact that the structure and function is comparable and the research on humans is legally, ethnically and medically extremely sensitive. Generally, the cardiac cycle can be described by an electrical and mechanical field. A repetitive electrical impulse occurring at the sinoatrial node located in the wall of the right atrium travels through the myocard of the atrium until the signal reaches the AV-node, which represents the connection between the atria and ventricles. The myocytes are connected via gap junctions and thus can transmit the electrical signal from cell to cell until each of them is triggered. The depolarization of the cardiac cells finally leads to the contraction of the muscle cells and generates the pumping function. This is known as the excitation-induced depolarization and contraction of cardiomyocytes. But also a stretch-induced opening of ion channels can cause depolarization. This leads to a strong coupling of the mechanical and eletrical field. In this study, we investigate the influence of the strongly coupled excitation-contraction problem on the fibrillation behaviour. The morphology

of the heart is represented by a rule based helical alignment of fibres. Our computational model is constructed from a 3D geometry of a rat heart based on MRI images provided by the Pediatric Cardiology in Erlangen. The phenomenological Aliev-Panfilov model for the non-oscillatory cardiac muscle cells and the Holzapfel-Ogden model for the passive mechanics of the cardiac tissue are embedded in a monodomain environment through the active stress approach. The results are illustrated by means of two- and three-dimensional examples of re-entrant spiral and scroll waves as well as ventricular fibrillation on MRI based data sets.

On the electro-chemo-mechanical modelling of stomach smooth muscle contraction

Lisa Klemm (*Technische Universität Braunschweig, Germany*) 16:50
Melanie Bauer (*Technische Universität Braunschweig, Germany*)
Enrique Morales (*Technische Universität Braunschweig, Germany*)
Robert Seydewitz (*Technische Universität Braunschweig, Germany*)
Markus Böl (*Technische Universität Braunschweig, Germany*)

The stomach is a J-shaped hollow organ in the gastrointestinal tract which undergoes large deformations during the ingestion of a meal. Its functions are the storage of food in the proximal half and its mixing and transport in the distal half, making the food suitable for further processing in the intestine. These tasks are performed by motoractivity of the smooth muscles in the stomach wall, whose failure can lead to several diseases, like gastroparesis.

A three-dimensional model of the gastric smooth muscle contraction, which is based on the electrical, chemical, and mechanical field, is presented. The electrical activation of the smooth muscle cells (SMC) due to pacemaker activity of interstitial cells of Cajal (ICC), the calcium dynamic in the SMC, and the force generation are coupled with an additional mechano-electrical feedback-mechanism, simulating the mechanical response of the SMC due to stretch of the stomach wall. In this way the typical peristaltic contraction waves, which can be observed in the antrum, have been well replicated in simulations performed on the tissue strip level as well as on the whole organ level.

Aside from the modelling, passive biaxial tensile tests in different regions and layers of the stomach wall have been realised, as well as histological researches to determine the fibre orientations and thicknesses of the stomach wall in dependence of the region. From these tests it can be concluded that the stomach wall is a highly inhomogeneous material.

Active-strain electromechanics for the computational modelling of gastric peristalsis

Sebastian Brandstaeter (*Technical University of Munich, Germany*) 17:10
Sebastian L. Fuchs (*Technical University of Munich, Germany, Hamburg University of Technology, Germany*)
Alessio Gizzi (*Campus Bio-Medico University of Rome, Italy*)
Roland C. Aydin (*Helmholtz-Zentrum Geesthacht, Germany*)
Christian J. Cyron (*Hamburg University of Technology, Germany, Helmholtz-Zentrum Geesthacht, Germany*)

Many of the stomach's physiological functions like mixing, grinding and propulsion of chyme rely on periodically propagating contraction waves termed gastric peristalsis. In part, gastric peristalsis is controlled by so-called slow waves: synchronized propagating bioelectrical waves initiated unintermittedly by interstitial cells of Cajal (ICC) of the gastric electrophysiological system. The diffusive spreading of slow waves to the surrounding tissue depolarizes smooth muscle cells (SMCs) initiating complex multiscale activation-contraction mechanisms that result

in a synchronous contraction. Therefore, the interplay between ICC and SMCs is essential for reproducing gastric peristalsis.

We present a constitutive framework for the phenomenological modelling of the electromechanical system underlying gastric peristalsis [1]. The framework explicitly incorporates the description of the electrophysiological system coupled to active smooth muscle contractility and passive mechanical tissue behaviour. The electrophysiological system is described with a phenomenological model by a total of four state variables, i.e., a set of two variables per cell type (ICC and SMCs). The cells' electrical activity is modelled by the same system of partial differential equations, differing only in the choice of parameter values, while, at the continuum scale, the electrophysiological system is represented by two coupled monodomain formulations [2]. Smooth muscle contractility is described by an active-strain finite elasticity approach while the passive mechanical behaviour is accounted for via a hyperelastic material formulation [3].

In a numerical convergence analysis, we analysed the influence of time step size and mesh size on the conduction velocity of the slow waves. By means of numerical experiments, we show the importance of the spatial distribution of ICC for entrainment and propagation of gastric slow waves and the consequential formation of stable ring-shaped peristaltic contraction waves both in physiological and pathological scenarios. The suitability of the proposed computational framework for large scale in-silico analyses of gastric electromechanics in health and disease is demonstrated on a set of simplified model geometries.

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Simulating electromechanical delay by using a multi-scale model of the muscle-tendon complex

Laura Schmid (*University of Stuttgart, Germany*)

17:30

Thomas Klotz (*University of Stuttgart, Germany*)

Tobias Siebert (*University of Stuttgart, Germany*)

Oliver Röhrle (*University of Stuttgart, Germany*)

Skeletal muscles can be voluntarily controlled by the somatic nervous system and thus enable motion, force production, and provide joint stability. Thereby, the time lag between the neural stimulation of a muscle and the onset of force production is known as electromechanical delay (EMD). In the context of applied physiology, a detailed understanding of the factors influencing EMD is supposed to contribute to the development of treatment strategies for ankle instability. While experimental studies suggest that EMD is dominated by the mechanical behavior of tendon tissue, the exact contribution of additional factors like the mechanical muscle properties, excitation-contraction-coupling (ECC), action potential propagation or neural control remains elusive. In this context, simulations enable numerical experiments in a controlled environment, in which the influence of single phenomena on EMD can be evaluated. The only simulation study analyzing EMD is based on Hill-type muscle models [1] and can not resolve spatial effects like the propagation of action potentials. Therefore, the aim of this work is to develop a three-dimensional multi-scale model that is capable of simulating EMD in a muscle-tendon system.

In detail, the continuum mechanical multi-scale model of Heidlauf & Röhrle [2] is modified by including tendinous tissue. Thereby, both the passive mechanical muscle and the mechanical tendon properties are described by a hyperelastic Ogden-type material. The corresponding material parameters are fitted to experimental data of the rat tibialis anterior muscle and the affiliated tendon [3]. The model is implemented in OpenCMISS and EMD is examined during variable conditions to quantify the impact of mechanical tissue properties, action potential propagation, ECC and neural control.

Throughout all applied stretches a characteristic shape of the EMD-stretch curve is obtained, i.e., EMD decreases with increasing stretch up to a stretch of 1.3 from where a slight increase in EMD is observed. Omitting the tendon leads to a different shape of the EMD-stretch curve, emphasizing the major contribution of the mechanical tendon properties on EMD. Further, it is found that EMD is highly sensitive to the rate of force production, pointing out the importance of ECC and neural synchronicity. In contrast, the propagation velocity of the action potential is found to have minor influence on EMD.

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Towards overcoming the bottleneck of optimizing control parameters in finite element active human body models

Oleksandr V. Martynenko (*University of Stuttgart, Germany*)

17:50

Katrin Stollenmaier (*University of Tuebingen, Germany*)

Carola Ender (*University of Stuttgart, Germany*)

Fabian T. Neininger (*University of Stuttgart, Germany*)

Syn Schmitt (*University of Stuttgart, Germany*)

Daniel F.B. Haeufle (*University of Tuebingen, Germany*)

Active finite element human body models (FE aHBMs) are now more and more frequently being used for the design and test of automotive safety systems. Especially for simulations of the motor vehicles accident pre-crash phase, where active human movement is present and significant. Such models are capable of accounting for dynamic human behaviour and reflexes by incorporating bio-inspired muscle controllers that produce stimulation signals to all active muscle elements. This introduction of active muscle elements and the corresponding controller code dramatically increases simulation runtime (up to five times), which is of crucial value to the entire research and development process of a new vehicle. Thus, new methods for reducing the runtime of the FE aHBMs simulations are required.

In previous works, we presented a muscle control algorithm for FE aHBMs based on intermittent equilibrium point control. The approach was implemented in FE LS-DYNA software code as a hybrid controller to dynamically set the activation of specific muscle elements with an “Extended Hill-type Muscle Model” material. This method demands a definition of optimised parameters for the open-loop central nervous system command and the closed-loop reflex signals before running the simulation. Tuning these parameters is currently the bottleneck of using this bio-inspired control approach in FE aHBMs.

We propose to determine these parameters in a reduced multibody model. The advantage of the MB model is its computational efficiency. We implement the same control approach in the MB model and use this to determine the parameters. This contribution describes the method of hybrid controller parameters approximation for desired equilibrium points using a MB model of the human arm with subsequent transfer to a fully deformable FE model. This approach

allows to reduce the simulation time needed for the controller parameters tuning and promises the feasibility of such bio-inspired motor control models in full FE aHBMs in the near future.

A cable model for accurate and efficient forward-dynamic musculoskeletal system simulation

Michael Helmut Gfrerer (*TU Kaiserslautern, Germany*)

18:10

Bernd Simeon (*TU Kaiserslautern, Germany*)

The aim of this contribution is to present a cable model for skeletal muscles within a musculoskeletal system simulation. Following the state of the art, we represent the skeletal system as a rigid multibody system. However, in typically musculoskeletal system simulation the muscle paths are modeled as straight lines between attachment points and via-points or as 1d curves wrapping around obstacles. Furthermore, the muscle force is computed from a lumped parameter model. In contrast to this, we treat the muscles as 3d bodies following the dynamics of nonlinear continuum mechanics. We employ an active stress approach. The active stress is modeled by a Huxley model, whereas the passive response is modeled by an incompressible Kelvin-Voigt material law. In order to reduce the computational cost the kinematics of the muscles is described by the position of the centerline only. Furthermore, we neglect bending and shear stresses. Nevertheless, the thickness change during the deformation is included in the contact between bones and muscles. We apply our framework to conduct a dynamic-forward simulation of a simple arm model.

S02.06 | Biomechanics

Date: February 21, 2019

08:30-10:30

Room: HS 01

Parametric investigation of permeability of vertebral bone assuming a regular microstructure

Zubin Trivedi (*University of Stuttgart, Germany*)

08:30

Christian Bleiler (*University of Stuttgart, Germany*)

Arndt Wagner (*University of Stuttgart, Germany*)

Oliver Röhrle (*University of Stuttgart, Germany*)

Percutaneous vertebroplasty is a commonly used practice for restoring the structural strength of vertebral bones affected by osteoporosis by injecting polymethylmethacrylate into the cancellous structure of the bone. However, a lack of predictability of the cement infiltration pattern often leads to cement leakage outside the bone, which may lead to complications like pulmonary embolisms. The infiltration behaviour of the cement depends on many factors, e.g. cement viscosity, its rheological characteristics, bone porosity, and the internal geometry of the microstructure, thus, making it a complex problem. Towards this objective, a study is carried out in the present work by assuming the vertebral bone to be a porous medium with a regular microstructure. The permeability of such a microstructure is investigated from a parametric perspective.

As a starting point, a method is first developed to determine the permeability of a regular microstructure using two models in tandem: a pore-scale model and a REV-scale model. The pore-scale model is created and solved using CFD solvers on ABAQUS, while the REV-scale model is solved using the Theory of Porous Media (TPM). Comparing the outputs, such as the seepage velocity of these two models, allows translating the pore-scale characteristics of the microstructure of the porous medium to the macro-scale quantities, e.g. the permeability of the microstructure. The results obtained using this two-pronged approach were found to be of the expected order of magnitude.

The method was used to carry out a parametric investigation by assuming the microstructure to be made of uniform-sized spheres, wherein the packing structures and the radii of spheres were varied to tune the parameters porosity and the specific surface area respectively in a controlled manner. The change in the permeability with each of these parameters was recorded and compared with the semi-empirical Kozeny-Carman relation for validation. While the trends in the variation of permeability were found to be matching, the accuracy of the absolute values was found to be subject to the value of tortuosity used in the Kozeny-Carman relation. Using the values of tortuosity for packed beds of spherical or quasi-spherical particles by imaging techniques from external works, most of the numerical results match with those obtained from the Kozeny-Carman relation with the difference in the range of 15 - 20 %.

Multiscale modeling provides differentiated insights to fluid flow-driven stimulation of bone cellular activities

Sarah-Jane Estermann (*Vienna University of Technology (TU Wien), Austria, Karl Landsteiner Universität für Gesundheitswissenschaften, Austria*)

08:50

Stefan Scheiner (*Vienna University of Technology (TU Wien), Austria*)

Both the shape of bone organs and the micro-architecture of bone tissue are significantly influenced by the prevailing mechanical loading. In this context, several of the most striking and hence also most debated issues relate to the question how bone is actually able to sense and process its mechanical environment. Among other stimuli, it has been hypothesized that the macroscopic mechanical loading induces pressure gradients in the pore spaces of bone tissue, and that these pressure gradients lead to fluid flow exciting the cells that are located in the pore spaces. Since in vitro tests confirmed that cells subjected to the flow of the surrounding fluid indeed respond in form of altered expression activities, the scientific community has in large part embraced the "fluid flow-hypothesis". However, direct experimental evidence as to the actual occurrence of sufficiently fast fluid flow (in order to reach the cell responses observed in vitro) has not been attained so far. In this paper, a multiscale modeling strategy is presented (inspired by the well-established concept of continuum micromechanics), allowing for upscaling (or homogenization) of the fluid flow contributions in the canalicular, lacunar, and vascular pores in terms of a corresponding macroscopic permeability of bone tissue. The same model also allows for proceeding the opposite way, namely for downscaling macroscopically acting pressure gradients to the pore levels. Thus, physiologically relevant mechanical loading conditions can be related straightforwardly to the correspondingly arising pore-scale pressure gradients, and, through considering the resulting pressure gradients in suitable transport laws, also to related fluid velocities. When comparing the such computed fluid velocities with the fluid velocities that were shown to efficiently excite bone cells in vitro, it turns out that pressure-driven fluid flow in the canalicular pores is probably not a potent mechanical stimulus for osteocytes, whereas fluid flow in the vascular pores may indeed reach the required fluid velocities and hence excite the therein residing osteoblasts, osteoclasts, and bone lining cells. In conclusion, the work presented in this thesis provides important, unprecedented insights as to the observation scale-specific cellular mechanosensation in bone.

Numerical simulation of function-perfusion processes in the human liver using the theory of porous media

Lena Lambers (*University of Stuttgart, Germany*)

09:10

Tim Ricken (*University of Stuttgart, Germany*)

Matthias König (*Humboldt University Berlin, Germany*)

The liver is the key metabolic organ in the human body and responsible for essential functions like glucose homeostasis or fat storage. A central role of the liver is to detoxify the blood from

toxic substances and drugs which in excess can cause damage to the liver structure, ultimately leading to acute liver failure.

The liver function can be impaired by various liver diseases e.g. non-alcoholic fatty liver disease (NAFLD). A clinically relevant example of impairment of liver structure and perfusion, and consequently function, is hepatotoxicity from paracetamol overdose. To simulate these complex structure-function-perfusion processes in the liver mathematical models are essential, see [1].

The developed model is an extension of a previously published work, where a multicomponent, poro-elastic multiphasic and multiscale function-perfusion approach based on the Theory of Porous Media (TPM, see [2], [3]) was presented, cf. [4]. The model is capable of simulating fat and paracetamol metabolism in dependence on hepatic perfusion.

Since the liver has a complex and hierarchical organized structure, a scale bridging approach is required. The complete organ consists of so called liver lobules with an anisotropic blood flow via the sinusoids (slender capillaries between the periportal field and the central vein). In order to reduce computational effort resulting from the complex liver micro structure, we use a multicomponent mixture theory based on the TPM to describe the lobule scale.

The computational model consists of a tetra-phasic body, composed of a porous solid structure representing healthy tissue, necrotic tissue, fat tissue with the ability of growth and deplete and a liquid phase representing the blood.

The phases consist of a carrier phase, called solvent, and solutes, representing microscopic components e.g. nutrients or paracetamol, solved in the solvent.

The metabolism of paracetamol is performed by liver cells, called hepatocytes, which are located along the sinusoids. To calculate the metabolic processes, e.g., production of the hepatotoxic compound NAPQI, and to describe the production, utilization and storage of the metabolites on the cellular scale, an embedded set of coupled ordinary differential equations (ODE) is used.

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[2] DE BOER, R. [2002], Theory of porous media: highlights in historical development and current state

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[4] RICKEN, T., ET AL. [2015], Biomech. Model. Mechanobiol. 14, 515-536

On osmotic pressure and damage in hyperelastic biphasic fiber reinforced articular cartilage

Franziska Egli (*University of Stuttgart, Germany*)

09:30

Tim Ricken (*University of Stuttgart, Germany*)

As part of the connective tissue, articular cartilage is an extremely important component to ensure low-friction performance of the human musculoskeletal system. Cartilage is a complex multi-phase material consisting of a collagen fiber-reinforced porous solid which is saturated by a liquid phase. The mechanical properties are particularly influenced by the highly anisotropic and inhomogeneously distributed collagen fiber network and its interaction with the isotropically distributed proteoglycans. The electrically negative charged proteoglycans generate an electrical gradient which in turn causes an osmotic negative pressure. This leads to mechanical prestressing of the collagen fibers which reduces the total pressure on the cartilage matrix.

Osteoarthritis is a very common joint disease, mainly affecting older people. In the course of the disease a change in the composition of proteoglycans can be observed [1] which reduces the osmotic pressure. This leads to an increased abrasion followed by defibrination of the collagen fibers [2] and finally to a reduced tensile strength and viscoelasticity in fiber direction.

In order to better predict and thereby, if possible, avoid the damage processes that occur, a biphasic model based on [3] will be developed. Therein, the Theory of Porous Media [4,5] is

chosen for homogenization. The model deals with an incompressible poroelastic solid matrix reinforced with collagen fibers and an incompressible pore fluid. To determine the true stress-free reference configuration, the influence of osmotic pressure must be considered [6]. Taking the age-related degeneration process into account, the model is furthermore extended by a damage expression based on a continuum approach.

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[6] WANG, X. ET AL. [2018], "On incorporating osmotic prestretch/prestress in image-driven finite element simulations of cartilage", *Journal of the Mechanical Behavior of Biomedical Materials*.

Stability of crack growth in anisotropic materials at finite strains

Jakob Eckmann (*Graz University of Technology, Austria*)

09:50

Osman Gültekin (*Graz University of Technology, Austria*)

Gerhard A. Holzapfel (*Graz University of Technology, Austria, Norwegian University of Science and Technology, Norway*)

One of the central tasks in medical monitoring and risk assessment is the prediction of rupture in soft biological tissues. Nowadays, most criteria for surgeries are geometry-based and modern imaging techniques are used to define vulnerable plaques or aneurysms. These criteria often lead to unnecessary surgeries or fail to predict rupture. Therefore, the finite element analysis of patient-specific data is an important task in order to help surgeons in the decision making process. Thus, developing valid rupture criteria for fibrous biological tissues and their computer implementation are of fundamental interest.

The present study uses the anisotropic crack phase-field approach to fracture developed by Gültekin et al. [3, 4] on the basis of the work of Miehe et al. [1]. The model expands the sharp crack topology into a three-dimensional problem, which leads to a continuous transition of undamaged material to damaged one. Additionally, the crack prediction can be influenced by an anisotropy parameter, which prescribes the crack path depending on the material model used in the continuum mechanical framework.

In the current study, two different constitutive models were used to investigate the stability of the given rupture criterion: the first one was the model proposed by Holzapfel et al. [2] for anisotropic materials; the second one is a slightly modified version, which uses a Taylor series expansion for the anisotropic term of the aforementioned model, alleviating numerical issues associated with high values of the mentioned anisotropy parameter by relaxing the exponential expression.

Finally, a benchmark problem was performed for both models and comparisons were made with regard to the stability of the two different simulations. To further validate the approach, force-displacement curves and the resulting crack path were investigated and compared to each other.

The modified model will be used to simulate the atherosclerotic rupture of a diseased artery during supra-physiological blood pressure.

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Quantification of microdamage formation during fatigue testing of individual trabeculae

Julia-Theresa Fischer (*TU Wien, Austria*)

10:10

Martin Frank (*TU Wien, Austria*)

Philipp J. Thurner (*TU Wien, Austria*)

Osteoporosis is listed as one of the 10 most important diseases, according to WHO. Diagnosis of osteoporosis is limited to a quantitative classification of bone mineral density (BMD), whereas bone quality remains unknown. It has been shown that a decrease in bone quality is directly linked to an accumulation of microdamage, eventually leading to osteoporotic fractures. Hereby, regions containing mainly trabecular bone are major sites of osteoporotic fractures. So far, fatigue tests of trabecular bone were limited to mm-sized bone cores, making it challenging to separate structural influences from the actual microdamage behavior at the material level. However, microdamage characterization at this level (individual trabeculae) is necessary to minimize geometric influences arising from diseases, age or anatomic sites. In a previous study [1], a tensile test for individual trabeculae was successfully developed and a mechanical characterization of trabecular bone at the material level was performed. First, this test set-up allows testing of samples close to a physiologic environment (in a buffer solution) and at a defined stress state. Second, the test set-up allows a throughput of 10 samples per week, which is necessary because of the rather high inter-sample variability. Goal of the present study was to extend the test protocol for fatigue loading to induce microdamage. Samples were tested for 1500, 2100 and 3000 cycles, without fracturing them. Differences in sample geometry were accounted by adjustment of pre-load. Before testing, samples were stained with Alizarin Red, to visualize pre-existing microdamage. After testing, samples were stained with Calcein for detecting induced microdamage. Sequentially, samples were embedded in epoxy, ultra-milled and polished for high-quality microdamage visualization. Microdamage was observed with a confocal laser microscope for visualization of the actual 3D damaged volume and either classified as diffuse microdamage or linear microcracks. As expected, an increasing number of test-cycles resulted in a significant ($p > 0.05$) accumulation of microdamage. Hereby, damage density of diffuse microdamage was significantly ($p > 0.05$) larger than the one of linear microcracks. Interestingly, the number of linear microcracks decreased from 2100 to 3000 cycles, suggesting that they fuse with each other or with diffuse damage areas. These findings demonstrated that microcrack growth correlated with cycle number at the material level of trabecular bone, for the first time. The developed test protocol can be used in future studies to compare microcrack formation and growth in healthy and osteoporotic patients.

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S02.07 | Biomechanics

Date: February 21, 2019

14:00-16:00

Room: HS 01

Medical images registration with finite elements and mechanical regularization

Martin Genet (*École Polytechnique, France*)

14:00

Image processing, in particular motion tracking, is playing an important role in biomedical engineering and in other domains such as materials and mechanical engineering. However, despite important progress made in the past decades, robustness, efficiency and precision of the existing methods must still be improved to translate them into medical and engineering applications [1]. Equilibrated Warping is a novel image registration approach, based on the finite element method and the equilibrium gap regularization [2]. The finite element method is used to formulate the image registration problem, i.e., to find the displacement field that best match the source and target images, allowing to ensure some regularity to the solution. However, because of image limited resolution and noise, this problem is ill-posed, and requires regularization. The equilibrium gap regularization essentially penalizes any deviation from the solution of a hyperelastic body in equilibrium with arbitrary loads prescribed at the boundary [3]. It thus represents a regularization with strong mechanical basis.

In the presentation, I will first describe the consistent formulation, linearization and discretization of the regularized image registration problem. On simple synthetic images examples, I will provide first elements of validation, and show that the equilibrated warping method is effective and robust: regularization strength and image noise have minimal impact on motion tracking. Then, I will provide further elements of validation, and show that equilibrated warping compares very well with other image registration methods on a public cardiac motion tracking challenge data [1], on both cardiac Magnetic Resonance (MR) and Ultrasound (US) images. I will finally show results of the equilibrated warping method applied to in vivo tagged (3D CSPAMM) and untagged (CINE) cardiac magnetic resonance images of a healthy volunteer: the method allows to extract main deformation features of the left ventricle (radial thickening, circumferential and longitudinal shortening, ventricular twist), as well as finer features of deformations.

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Data-driven constitutive modeling of patient-specific cartilaginous tissue

Kevin Linka (*RWTH Aachen University, Germany*)

14:40

Mikhail Itskov (*RWTH Aachen University, Germany*)

Sven Nebelung (*RWTH Aachen University, Germany*)

Daniel Truhn (*RWTH Aachen University, Germany*)

Osteoarthritis is strongly associated with a degeneration of cartilaginous tissue, which, in turn, is accompanied by tissue softening. One promising non-invasive approach towards its detection

appears to be an assessment of multiparametric magnetic resonance (MR) imaging. However, so far, there is no reliable correlation between the exact tissue properties and the multiparametric MR image mapping. In this contribution, we developed a constitutive framework in order to inform a cartilage model by sample-specific multiparametric MR maps (T1, T1 ρ , T2 and T2*) generated by a clinical 3.0-T MR imaging system. The model predictions of individual patients were fitted against their sample-specific stress responses by enforcing a global set of material parameters. Accordingly, we obtained suitable relations between the specific MR maps and the biomechanical properties. These relations serve as an input for the proposed constitutive law in order to predict the individual stress response of the tested cohort.

Validation of aortic wall motion measurement by 4D ultrasound and effects of measurement uncertainty on inverse identification of the wall's constitutive behavior

Christopher Blase (*Frankfurt University of Applied Sciences, Germany*)

15:00

Wojciech Derwich (*Goethe University Hospital, Germany*)

Thomas Schmitz-Rixen (*Goethe University Hospital, Germany*)

Claus-Peter Fritzen (*University of Siegen, Germany*)

Armin Huß (*Frankfurt University of Applied Sciences, Germany*)

Andreas Wittek (*Frankfurt University of Applied Sciences, Germany, University of Siegen, Germany*)

Time-resolved three-dimensional ultrasound combined with speckle tracking algorithms (4D ultrasound) is a non-invasive medical imaging technique that provides full field displacement data of aortic and aneurysmal wall motion in vivo. Combined with inverse techniques to identify the parameters of an orthotropic and nonlinear elastic constitutive equation, this data type has the potential to overcome known limitations in the identification of the individual constitutive behavior of the human aortic and aneurysmal wall in a clinical setting. We have developed an in vivo Finite Element Model Updating (FEMU) approach to determining individual material properties and the load free configuration of human aortae and AAA based on in vivo 4D ultrasound full field strain measurement.

In an in vitro validation study, we have assessed the agreement of 4D ultrasound measurement of aortic wall motion with an optical reference measurement and the reproducibility (test-retest reliability) of 4D ultrasound measurement results. Compared to the reference, 4D ultrasound measurement did not show any systematic error. Random error of local displacement measurement was $IQR = 0.21$ mm in propagation direction of the ultrasound signal and $IQR = 0.18$ mm orthogonal to the propagation direction. The 95% confidence interval of local strain measurement for tissue segments with a size of about 1.5×1.5 mm was determined to be $\pm 2.1\%$. From repeated measurement and postprocessing of 5 different inflation-extension load cases of a porcine aortic sample an intraclass correlation coefficient of $ICC(1,1) \geq 0.90$ was found for the measurement of local diameter, diameter change and circumferential strain.

In a numerical verification experiment, we have examined the effect of the identified measurement uncertainty on the results of the inverse identification of the constitutive parameters and the load free geometry. Assuming an arbitrary but reasonable “master” constitutive behavior and diastolic and systolic blood pressure, data comparable to the clinically available 4D ultrasound full field strain measurements of wall motion were generated numerically. Random error as identified in the validation study was superimposed on the generated strain field data and these data were used as input to the inverse FEMU approach. The Hausdorff distance of the identified load free geometry was 0.3 mm, stress-stretch curves of the identified constitutive behavior along three characteristic load paths showed good agreement with the “master” material ($R^2 \geq 0.79$).

An efficient solver for CT based nonlinear microFE simulations of trabecular structures

Monika Stipsitz (*TU Wien, Austria*)

15:20

Dieter H. Pahr (*TU Wien, Austria, Karl Landsteiner Private University of Health Sciences, Austria*)

Computer tomography (CT) becomes a widely used non-destructive method to image micro-structured materials like bone. Simulation models generated from this uCT images - so called micro finite element (uFE) models - have resolutions of around 15-30um and allow studying the failure mechanisms at the micro-level. The high resolution results in large uFE models (1-2000 mio DOFs), which require efficient parallel solvers. The open source solver ParOSol [1] was designed for such tasks but is limited to linear problems. In this work, a nonlinear extension - ParOSolNL - is presented and applied to capture the apparent behavior of trabecular biopsies.

Methods

The linear-elastic uFE solver ParOSol was extended to include damage based material nonlinearity. The simple material model is able to capture material degradation and material failure via a scalar damage variable. The tension-compression asymmetry of bone tissue is taken into account via asymmetric damage onset stresses. The material parameters are identified using CT imaged trabecular bone biopsies from different body locations, showing a variety of different densities. Finally, 21 trabecular samples were simulated under compression or tension and compared to experimental results obtained by [2].

Results

Good agreement between the nonlinear simulations and the experiments was found in the apparent stress-strain curves of the trabecular biopsies. Linear regression analysis shows that the apparent modulus, apparent 0.2%-offset yield stress and ultimate stress are highly correlated between the experiments and the simulations. The failed regions obtained in the simulations look plausible; showing diffuse damage regions as well as distinct fractures. The FE models have 3-15 mio DOFs and resulted in average physical simulation times of 1.2 hours using 28 CPUs.

Conclusion

Although a very simple nonlinear material model and solving algorithm is used, the apparent behavior of trabecular biopsies can be captured quite well. The local failure regions look reasonable; however, the reliability of local results needs to be further investigated. Additionally, it has been shown that ParOSolNL can be applied to whole bone structures with sufficiently high resolution. Thus, we hope that ParOSolNL will enable more insight into the failure mechanism of bone structures.

References:

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Histology-based semi-automated 3D reconstruction and simulation of skeletal muscle tissue

Ramachandra Kuravi (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zurich, Switzerland*)

15:40

Alexandra Oswald (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zurich, Switzerland*)

Kay Leichsenring (*TU Braunschweig, Germany*)

Markus Böl (*TU Braunschweig, Germany*)

Alexander E. Ehret (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zurich, Switzerland*)

This contribution deals with the generation of 3D finite element models from histological sections of skeletal muscle. In addition to models obtained through manual segmentation from image stacks with varying numbers of sections, a semi-automated procedure is presented that strongly reduces the time and the effort of segmentation. The algorithm is based on deforming the single histological sections of the stack in order to match fibres on different layers, and therefore accounts for the continuity of muscle fibres through the tissue. The thus created fibre and extracellular matrix (ECM) sections are meshed and furnished with non-linear anisotropic material properties. The constitutive models that describe these properties of muscle fibres and ECM are separately parametrised by means of tensile test data on skinned muscle fibres [1] and new experimental data on decellularised muscle samples, respectively. The principal directions of anisotropy, i.e. the local directions of muscle fibres and the spatial orientation of the ECM assumed to wrap the fibres, are computed from an intermediate step, exploiting an analogy with steady state diffusion [cf. 2]. Based on this structural information, on the parametrised models and on the corresponding volume fractions of ECM and muscle fibres, the response of cuboid samples of muscle tissue in semi-confined compression tests is predicted in multiscale simulations and shows excellent agreement with experimental data [3].

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S02.08 | Biomechanics

Date: February 22, 2019

08:30-10:30

Room: HS 01

AFM-based microbeam bending of human cortical bone lamellae from the femur midshaft

Vedran Nedelkovski (*TU Wien, Austria*)

08:30

Orestis G. Andriotis (*TU Wien, Austria*)

Rainer Hahn (*TU Wien, Austria*)

Paul Heinz Mayrhofer (*TU Wien, Austria*)

Philipp J. Thurner (*TU Wien, Austria*)

Bone is a nanocomposite biological material with unique mechanical properties, owing to a complex hierarchical structure ranging from the nanoscale up to the macroscale. To better understand bone mechanics, investigation of mechanical properties of different structures on every hierarchical level and the way they interact is a promising approach. Although biomechanical testing of bone at the macroscale has been performed for over a century, investigation of microstructural features, such as individual lamellae, still remains a challenge. Focused ion beam (FIB) milling is an attractive technique for machining bone samples at the microscale, while avoiding inclusions of micro-porosities like lacunae and Haversian canals. So far, microbeams [1][2][3] and micropillars [4][5][6] from animal bone have been mechanically tested under bending with an atomic force microscope (AFM), or under compression with a conventional nanoindenter, respectively, either in dehydrated or rehydrated state. However, micro-scale experiments detailing mechanical properties of human bone have not been reported. Here we present an AFM-based microbeam bending method for micromechanical assessment of human cortical bone in both dehydrated and rehydrated state. FIB-machined microbeams from the femur midshaft of 4 male donors, aged 65-94y were bent with an AFM tip along the beam length [7], first dehydrated in air and then rehydrated in Hank's Balanced Buffer Solution (HBSS). Prior to this, the measurement setup was calibrated by bending FIB-milled Si microbeams of known stiffness utilising an indenter situated

within a scanning electron microscope. From the measured stiffness versus bone beam position data, bending moduli were obtained as a fit parameter. Values ranged (25.1-48.7) GPa in air and (7.3-19.1) GPa in HBSS. A decrease of bending modulus up to 5 times was observed for a single microbeam, suggesting a change in deformation mechanism upon rehydration. No significant change of bending moduli was observed with respect to age. Moreover, bending in air exhibited linear elastic behaviour, with same apparent loading and unloading stiffness, whereas in HBSS higher unloading stiffness was observed, suggesting dissipative deformation mechanisms during loading. The dissipated energy in rehydrated samples was calculated as the area between the loading and unloading curve, ranging from 0.093 to 0.655 pJ (i.e. 5.8-64.5% of the total energy) and was found to decrease with age. These preliminary findings suggest important implications of the role of water in the deformation mechanisms of bone, which in turn may play a role in decreased fracture toughness and increased fragility of bone with age.

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Hierarchical elastoplasticity of bone

Valentina Wittner (*TU Wien - Vienna University of Technology, Austria*)

08:50

Claire Morin (*Ecole Nationale Supérieure des Mines, Saint-Étienne, France*)

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

Bone is characterized by a hierarchically organized microstructure, exhibiting universal organizational patterns, whose "dosages", however, vary between different species, organs, and anatomical locations. This complex internal structure leads to a necessity of taking into account all hierarchical components - some of which behave plastic - in order to explain the overall elastoplastic response of bone.

A multiscale continuum micromechanics model is used to predict the resistance to failure under mechanical load - the bone strength - based on the mechanical properties and volume fractions of bone's three elementary constituents: mineral, collagen and water.

The hierarchical organization of bone is considered in terms of a micromechanical six-step homogenization scheme. Within this model, the sole source of elastoplasticity lies in mutual sliding between mineral phases. While the mineral is characterized by non-associated Mohr-Coulomb elastoplasticity, the collagen fails in a brittle manner, according to a Rankine-criterion. Upscaling of these processes from the nano- to the macroscale was made possible by a novel iterative variant of the so-called return-map algorithm.

The model is able to accurately predict the experimentally determined strength of bones of different species and anatomical locations tested in uniaxial tension and compression. Furthermore, the sequence of plastic events and the stresses and strains can be determined across all hierarchical levels, illustrating the influence of the specimen-specific bone composition, which is governed by the bone porosity and the mass density, on the overall mechanical behavior of the bone.

NURBS-enriched finite element formulation for frictional contact between bone and implant

Katharina Immel (*RWTH Aachen University, Germany, CNRS, Laboratoire Modélisation et Simulation Multi Echelle, France*) 09:10

Thang X. Duong (*RWTH Aachen University, Germany*)

Roger A. Sauer (*RWTH Aachen University, Germany*)

Vu-Hieu Nguyen (*CNRS, Laboratoire Modélisation et Simulation Multi Echelle, France*)

Guillaume Haiat (*CNRS, Laboratoire Modélisation et Simulation Multi Echelle, France*)

Cementless implants are widely used in orthopedic and oral surgery. However, failures still occur and may cause the debonding of the bone-implant interface. It remains difficult to predict implant failure since the underlying osseointegration phenomena, especially in terms of friction and adhesion, and their influence on the primary and secondary stability of the implant, is still poorly understood. This work presents a formulation that can model the frictional contact behavior between osseointegrated implants and bone tissue, based on [2, 4]. The proposed model distinguishes between static and dynamic friction, and accounts for adhesive debonding. Various transition functions between static and dynamic friction are used to model the decrease of friction due to debonding of the implant.

The formulation is validated with experimental and analytical results of the mode III cleavage of coin-shaped, osseointegrated, titanium implants [3]. Both, bone and implant, are modeled with a nonlinear Neo-Hookean material formulation and three-dimensional NURBS-enriched finite elements [1] are used to ensure accurate contact treatment.

Comparing the resulting variation of the torque as a function of the angle in the mode III cleavage experiment, the results of the friction model show a better agreement with the experimental results than the analytical model, especially for the initial slope and the peak of the torque curve.

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- [4] Roger A. Sauer and Laura De Lorenzis. “An unbiased computational contact formulation for 3D friction”. *International Journal for Numerical Methods in Engineering*, 101(4), 2015.

Towards physiological conditions in total knee arthroplasty by a bionics-inspired tibial implant design

Bernhard Eidel (*Universität Siegen, Germany*)

09:30

Ajinkya Gote (*Universität Siegen, Germany*)

Claus-Peter Fritzen (*Universität Siegen, Germany*)

Arne Ohrndorf (*Universität Siegen, Germany*)

Hans-Jürgen Christ (*Universität Siegen, Germany*)

In total knee arthroplasty (TKA) force is transmitted into the tibia by a combined plate-stem device along with cemented or cementless stem fixation. The present work analyzes this force transmission in finite element simulations with the main aim to avoid reported postsurgical bone density reduction as a consequence of a reduced tibial bone loading. In the numerical analysis different implant materials, stem/extension lengths and implant-to-stem interface conditions are considered, from a stiff, fully cemented fixation to sliding contact conditions with a low friction coefficient. The impact of these variations on bone loading changes are measured by (i) decomposing the total force into parts mediated by the plate and by the stem and by (ii) post-surgery strain energy density (SED) deviations. Based on a bionics-inspired perspective on how nature in pre-operative conditions carries out force transfer from the knee joint into the tibia, a modified implant-bone interface is suggested that alters force transmission towards physiological conditions while preserving the geometries of the standard plate-stem endoprosthesis design. As a result stress shielding is avoided almost completely, pre-surgery bone loading is preserved such that bone resorption is not likely to occur.

An experimental testing workflow for personalized osteosynthesis systems

Michael Roland (*Saarland University, Germany*)

09:50

Thorsten Tjardes (*Saarland University, Germany*)

Martin Reis (*Saarland University, Germany*)

Bertil Bouillon (*Saarland University, Germany*)

Stefan Diebels (*Saarland University, Germany*)

A personalized approach to fracture therapy necessitates the integration of knowledge and techniques from mechanics, orthopedic trauma surgery and computer science. Merging the relevant knowledge of these disciplines can lead to the development of less invasive, individually tailored treatment approaches comprising the surgical technique and the implant used.

Focusing on the case of distal tibia fractures, a new setup for a more realistic experimental testing of osteosynthesis systems is presented. Therefore, the experimental workflow is organized as follows: (1) starting point is a testing device to produce predefined tibia fractures, (2) the fractured lower extremities will be treated by an orthopedic trauma surgeon and (3) tested in a second testing device simulating the forces acting during a normal step forward. The experiments are realized with fresh frozen human cadaveric specimen.

During the first step of the workflow, the main goal is the repeatability of the fractures with respect to the applied forces and moments. Before the procedure starts, computed tomography scans of the bones are performed and are used as basis for the simulations. After the fracture is produced, an orthopedic trauma surgeon treats the lower extremity with an osteosynthesis locking plate and a second computed tomography scan is executed to enhance the computational model. Thereafter, in the last step of the testing workflow, the treated tibia is clamped in the second testing device and a mechanical loading scenario is applied on the bone-implant-system. The loading scenario is based on the OrthoLoad database and is calibrated by the subject-specific data of the human cadaveric specimen. During the test, stresses and strains are gained via a

high-speed camera system combined with digital image correlation and several pressure and force measurements. This workflow allows a more realistic testing of tibia implants and gives information about the mechanical behavior of the fracture gap, like the interfragmentary move. The whole procedure can also simulated based on the performed tomograms combined with the CAD data of the implant and the screws. Therefore, the image stacks are segmented, the material parameters are assigned and passed to a meshing procedure. After that, finite element simulations are executed with respect to the testing parameters and protocols in order to validate and to verify the simulation process. Here, the investigation of the simulations is focused on the best possible match of the experiments and the achieved results.

S03 | Damage and fracture mechanics

Organiser: Andreas Ricoeur (*University of Kassel, Germany*)
Stephan Wulfinghoff (*Kiel University, Germany*)

S03.01 | Damage and fracture mechanics

Date: February 19, 2019
Room: HS 50

08:30-10:30

A phase-field model of brittle fracture for an isogeometric Reissner-Mindlin shell formulation

Georgia Kikis (*RWTH Aachen University, Germany*)

08:30

Marreddy Ambati (*TU Braunschweig, Germany*)

Laura De Lorenzis (*TU Braunschweig, Germany*)

Sven Klinkel (*RWTH Aachen University, Germany*)

One of the biggest challenges in fracture modeling is the correct physical description of fracture processes. Over the past decade, the phase-field modeling framework has gained a lot of attention, due to its proven ability to predict fracture phenomena. It has shown very promising results for a three dimensional solid formulation and has been extended to an isogeometric Kirchhoff-Love formulation in order to describe brittle fracture in plates and shells, see [1]. However, the Kirchhoff-Love theory only describes thin shells. For thick shells, the deformation behavior and subsequently the fracture behavior additionally depend on the transverse shear strains which are not present in the Kirchhoff-Love approach.

In this work, the phase-field fracture framework is extended to an isogeometric Reissner-Mindlin shell formulation [2]. In this approach, the shell is described using the midsurface and a director vector field for the thickness direction. Therefore, the phase-field is also defined only on the midsurface. In order to distinguish the cracking behavior in tension and compression, as proposed in [1], the spectral decomposition of the strain for the tension-compression split is done on the total strain, which varies through the thickness. The proposed method is tested for several numerical examples and compared to a three dimensional solid formulation and to the Kirchhoff-Love shell formulation in order to assess its accuracy.

References

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An FFT-based solver for brittle fracture on heterogeneous microstructures

Felix Ernesti (*Karlsruhe Institute of Technology (KIT), Germany*)

08:50

Matti Schneider (*Karlsruhe Institute of Technology (KIT), Germany*)

Thomas Böhlke (*Karlsruhe Institute of Technology (KIT), Germany*)

The description of material failure as an energy minimization problem, i.e., the Francfort-Marigo model [1], has been studied widely in recent years. The approximation of the crack surface as a

phase field, i.e., smeared interface, enjoys great popularity, as it allows describing fracture as a set of partial differential equations.

In numerical homogenization, FFT-based solution methods have been established over the past two decades [2]. Their purpose is to compute the overall response of a heterogeneous microstructure on a load and can be applied to a variety of nonlinear materials. The balance of momentum is reformulated as a Lippmann-Schwinger fixed point equation and discretized on a regular voxel grid. The benefits lie in a fast implementation and the possibility to use image data like cT-scans as input without further need for meshing. The iterative solution methods do not require any linearization.

This talk presents a combination of both methods. We derive a set of Lippmann-Schwinger equations that solve for extreme values of the Ambrosio-Tortorelli functional. The equations are discretized with a trigonometric collocation method. An alternating algorithm to solve the set of equations is presented and acceleration methods are discussed. Within this setting, no viscous damping for the material law is required.

With the introduced solver, we investigate the brittle behavior of different heterogeneous microstructures. Numerical tensile experiments with 2D spherical inclusions show the behavior of the solver. A numerical investigation on the crack surface through a 3D fiber reinforced composite shows the advantages of the former introduced methods.

[1] G. A. Francfort and J.-J. Marigo. Revisiting brittle fracture as an energy minimization problem. *Journal of Mechanics Physics of Solids*, 46:1319-1342, 1998.

[2] H. Moulinec and P. Suquet. A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Computer Methods in Applied Mechanics and Engineering*, 157:69-94, 1998.

Phase field modeling of interface effects on cracks in heterogeneous materials

Charlotte Kuhn (*Technische Universität Kaiserslautern, Germany*)

09:10

Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

One of the reasons why the phase field approach has become very popular for modeling fracture processes is that therein the entire evolution of fracture follows from energetic principles without the need for different criteria for crack initiation, nucleation, kinking or branching. Furthermore, these models allow for a straightforward numerical implementation with standard finite elements, since displacement jumps and stress singularities are avoided in these models. Consequently, phase field fracture models are now also used to model and simulate fracture of heterogeneous materials such as composites, where cracks may be arrested, deflected or bifurcated at interfaces between the different components of the composite material, resulting in complicated crack patterns. The crack propagation is not only controlled by the elastic and fracture properties of the bulk phases of the material but also by the properties of the interfaces in between. Thus, it is crucial to take these interface properties into account, and there are conceptually different approaches on how to integrate them into phase field fracture models. In [1] interfaces are modeled as zones of finite width with appropriately adjusted fracture parameters. Contrary, a combination with a cohesive type of modeling interface fracture is proposed in [2]. Another approach, which makes use of a new energetic formulation mixing bulk and cohesive surface energies, is proposed in [3]. In this work, interfaces are equipped with a fracture energy corresponding to the phase field fracture energy of the bulk phases in order to model the interface fracture properties. In the finite element implementation, the interfaces are modeled by means of surface elements without introducing additional degrees of freedom. The convergence behavior of the proposed model with respect to the sharp interface limit of the phase field fracture model as well as energy release rates during crack propagation are analyzed in numerical studies in order to verify the model.

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- [2] C.V. Verhoosel, R. de Borst: A phase-field model for cohesive fracture. Int. J. Numer. Meth. Engng 2013, 96:43-62
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A new framework to simulate fatigue fracture in brittle materials

Pietro Carrara (*Technische Universität Braunschweig, Germany*)

09:30

Marreddy Ambati (*Technische Universität Braunschweig, Germany*)

Roberto Alessi (*Università di Pisa, Italy*)

Laura De Lorenzis (*Technische Universität Braunschweig, Germany*)

Fatigue is a key phenomenon in mechanics, and is largely responsible for most structural failures. Despite the significance of the problem, most existing fatigue theories are based on empirical laws that lack of generality and predictive capabilities. In general, a framework that covers both the mechanics of monotonic fracture (including nucleation, propagation and failure) and the fatigue behavior reproducing the Palmgren-Miner law, the Paris law and the Wöhler curve with the transition between oligo-, low- and high-cyclic fatigue is still missing [1].

The present work aims at proposing a novel framework to model fatigue in brittle materials based on the variational phase-field approach to fracture. The standard phase-field free energy functional is modified similarly to [2] so as to allow the fracture toughness of the material to decrease as a suitable fatigue scalar history variable increases. The reduction rate is governed by a fatigue degradation function that acts as a fatigue constitutive equation and takes as argument only the fatigue history variable. The choice of both history variable and fatigue degradation function is very flexible, being subjected only to some general requirements to preserve the variational nature of the approach. In the present work, the fatigue history variable is assumed as the cumulated active part of the elastic strain energy density. Two definitions of the cumulated variable and two fatigue degradation functions are proposed, allowing to reproduce the major fatigue characteristics of different brittle materials. Depending on the specific choice, a maximum of three additional parameters is required.

Through the analysis of some numerical example we demonstrate the capability of the approach to reproduce the major features of the fatigue behavior including the crack nucleation, stable and unstable propagation phases. Also, the Paris law and the Wöhler curve are obtained naturally, while the Palmgren-Miner rule and the monotonic behavior are encompassed as special cases.

References

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Phase field modeling of dynamic brittle fracture of thin shells

Karsten Paul (*RWTH Aachen University, Germany*)

09:50

Christopher Zimmermann (*RWTH Aachen University, Germany*)

Kranthi K. Mandadapu (*University of California at Berkeley, USA*)

Thomas J.R. Hughes (*The University of Texas at Austin, USA*)

Chad M. Landis (*The University of Texas at Austin, USA*)

Roger A. Sauer (*RWTH Aachen University, Germany*)

The reliable prediction of structural defects has gained importance since requirements concerning robustness and safety are increasing. In phase field methods the damage region is smoothed and discontinuities in the geometry and solution are avoided. Based on Griffith's theory of brittle fracture, the partial differential equation (PDE) governing the phase field's evolution is found as the minimizer of an energy functional. The deformation of thin shells is characterized by the Kirchhoff-Love thin shell equation [2]. An energy split is introduced which accounts for stretching and bending to the fracture process separately. While the in-plane part is characterized by kinematical quantities living on the mid-plane of the shell, the bending terms are handled using a thickness integration. The coupled problem includes two nonlinear fourth-order PDEs defined on an evolving two-dimensional manifold. Since C1-continuity is required in the numerical solution, an Isogeometric Analysis (IGA) framework is used. The interface region is adaptively refined using locally refinable (LR) NURBS [1] that capture the diffusive character of the phase field correctly. A generalized-alpha scheme is employed for the temporal discretization [3]. The discretized coupled problem is solved within a monolithic Newton-Raphson scheme. Numerical examples are shown illustrating the behavior and interaction between surface deformation and crack evolution.

[1] C. Zimmermann, and R. A. Sauer, *Comp. Mech.* 60, 1011 (2017)

[2] T. X. Duong, F. Roohbakhshan, and R. A. Sauer, *Comput. Methods Appl. Mech. Eng.* 316, 43 (2017)

[3] M. J. Borden, C. V. Verhoosel, M. A. Scott, T. J. R. Hughes, and C. M. Landis, *Comput. Methods Appl. Mech. Eng.* 217-220, 77 (2012)

Peridynamic investigation of dynamic brittle fracture

Sahir Butt (*Ruhr Universität Bochum, Germany*)

10:10

Günther Meschke (*Ruhr Universität Bochum, Germany*)

In this study, we investigate the dynamic fracture process in amorphous brittle materials using 3D peridynamic analyses of dynamic crack propagation in PMMA plates subjected to quasi-static loads. This loading condition allows one to assume, that the crack will accelerate to a steady-state velocity and will continue propagating straight forward at a constant velocity. Dynamic crack instability and its effect on the fracture surface creation as well as the dissipated energy is analyzed numerically for cracks propagating at different velocities. Simulations reproduce many salient features of experimental observations, such as instabilities of crack occurring for cracks propagating above a certain critical velocity. It is shown from the simulations, that increasing crack velocity results in excessively repeated microbranching. An increased energy dissipation is also observed at higher crack velocities in the simulations, which correspond to the well known velocity toughening effect. The simulations also reproduce a limiting crack speed, which is below the theoretical limit, i.e. the Rayleigh wave speed.

Delta- and n-convergence, i.e. the effect of the peridynamic horizon and the mesh size on the fracture process respectively, is investigated for cracks propagating at different speeds. From delta-convergence study one can conclude, that the elastic wave dispersion properties have a

significant effect on the velocity of the macro-crack and subsequent velocity dependent dissipation mechanisms. Fracture patterns obtained using different peridynamic horizons are analyzed and a positive correlation is shown to exist between the microbranch spacing and the microbranch length.

Finally, the effect of the specimen geometry, i.e. specimen thickness and height, on crack dynamics is analyzed. These two dimensions of the specimen affect the crack dynamics in different ways. On one hand, the thickness of the specimen causes the crack dynamics to change because of the three dimensional effects. A single flat crack surface in a 3D plate has a curved crack front and the curvature of this crack front is governed by the thickness of the plate. This curvature increases the fully damaged zone, i.e. the length of the crack front, which results in a lower local dissipation rate. On the other hand, the height of the specimen affects the interaction of the stress waves reflecting from the boundaries. To this end, we carry out crack propagation simulations in PMMA specimens with different thickness and constant heights and vice versa.

S03.02 | Damage and fracture mechanics

Date: February 19, 2019

16:30-18:30

Room: HS 50

A variational phase field model for ductile fatigue

Stephan Teichtmeister (*University of Stuttgart, Germany*)

16:30

Roberto Alessi (*Sapienza University of Rome, Italy*)

In the recent years the phase field approach has proven to be quite successful in simulating complex fracturing in brittle as well as ductile materials. The potential of the method is underlined by extensions towards various coupled effects such as thermal- and diffusion-induced cracking. So far, the majority of these models are restricted to the case of monotonic loading. However, a key phenomenon that is responsible for most of the failures in structures is fatigue. Although, research on fatigue failure mechanisms was already done in the 19th century by August Wöhler, it is still a challenging topic, in particular from the modeling point of view. The circumstance, that experimental investigations on fatigue are expensive and time-consuming, underpins the necessity of a predictive and robust simulation tool.

In this presentation we will set up a variational phase field model that accounts for fatigue effects in ductile materials. Therein, the key idea is the construction of proper fatigue degradation functions, that reduce the material fracture toughness by elastic as well as plastic contributions. Thereby, we model a transition between the process of damage initiation and the process of damage evolution. The proposed model is able to describe low-cycle as well as high-cycle fatigue regimes. A key aspect of this work is a comparison of the model predictions with experimental data. In this connection, we also propose a new nonlinear combined isotropic-kinematic hardening law. Finally, the damage localization process in a bar under cyclic load will be discussed.

Application of higher-order strain gradient theories in the phase-field modelling of fracture mechanics

Daniel Juhre (*Otto von Guericke University Magdeburg, Germany*)

16:50

Resam Makvandi (*Otto von Guericke University Magdeburg, Germany*)

The simulation of crack propagation has always been a challenging task from a computational point of view. In the past, many mathematical and mechanical assumptions had to be taken into account to successfully simulate this process. The problem of tracking the sharp crack surface

was among the first issues which was alleviated by the introduction of phase-field models. The appearance of stress singularities near the crack tip in the classical continuum mechanics theory is considered to be another source of problem which makes the selection of proper mesh sizes for numerical models very cumbersome, and leads to unphysical results. In the presence of a singularity, the crack propagation starts earlier in problems with a finer discretization which is only natural considering that the strain energy density is higher and increases faster for smaller mesh sizes. Likewise, a loading which normally could not cause a crack to nucleate or propagate inside a structure, will do so in the numerical simulation due to over-estimated stresses. Therefore, it stands to reason that removing this singular field from the results is a very crucial step in achieving physically meaningful results. The goal of the current contribution is twofold: first, existing models are shown to exhibit a singular stress behavior, and second, a possible remedy is proposed based on the application of higher-order strain gradients.

Efficient phase-field modelling of fatigue crack propagation

Martha Seiler (*TU Dresden, Germany*)

17:10

Thomas Linse (*TU Dresden, Germany*)

Peter Hantschke (*TU Dresden, Germany*)

Markus Kästner (*TU Dresden, Germany*)

The phase-field method is an established approach to simulate brittle fracture, because it allows for the modelling of crack phenomena like initiation and branching. It has been applied to simulate fatigue fracture due to cyclic loading. Alessi et al. (EngFracMech 2018) use accumulated strain in order to reduce the fracture energy. However, fatigue failure comes along with high numbers of load cycles, so an explicit simulation of the load path is expensive, especially for inelastic material models. Therefore, time-efficient simulation methods are required.

In this contribution, we combine the phase-field method for brittle fracture [Miehe et al., CMAME 2010] with the notch strain concept [Seeger, Stahlbau Handbuch 1996], an empiric method to calculate the life span of components. In this way, we avoid the explicit simulation of the load cycles by executing a local cyclic damage calculation. Based on the accumulated fatigue damage, the critical fracture energy is degraded locally in order to describe the dissipation.

We can reduce calculation time further by using an elastic material model, since the notch strain concept provides a plastic revaluation of elastic stresses and strains [Neuber, JapplMech 1961]. Plasticity as the reason for fatigue crack propagation is thereby considered by cyclic stress-strain curves. The cyclic degradation of the material is characterised by standard strain-controlled Wöhler fatigue tests. Using numerical examples in 1D and 2D, it can be shown that the developed method is able to simulate fatigue crack initiation as well as propagation.

On phase field modeling in the context of cyclic mechanical fatigue

Christoph Schreiber (*Technische Universität Kaiserslautern, Germany*)

17:30

Charlotte Kuhn (*Technische Universität Kaiserslautern, Germany*)

Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

Cyclic mechanical fatigue is a very important phenomenon, which has to be well-considered for the design of many technical structures. However, although this phenomenon is known since the middle of the 19th century, corresponding numerical tools are still rather less incorporated within development processes.

The framework of phase field modeling provides several benefits for the numerical simulation of a crack path. The method was so far applied to quasi static fracture in brittle and also in ductile materials. Models incorporating inertia effects (dynamic fracture) or effects caused by an anisotropy of the fracture resistance were also developed. However, the field of phase field fatigue

crack modeling is still in the beginning. Within this talk a phase field model that enables the simulation of the evolution of cracks, driven by cyclic mechanical fatigue is presented. Integrating an additional component in the total internal energy formulation, accounting for the irreversible processes caused by cyclic loading and unloading, leads to crack extension even for small load amplitudes. The model's governing equations including the new driving force mechanism in terms of the damage state occurring at a specific location that connects the evolution of the crack phase to a number of load cycles with a certain load amplitude are derived. It is shown that the formulation is consistent with respect to a monotonically increasing load function. Numerical examples are discussed and results of fatigue crack growth simulations utilizing the presented model are compared to phenomenological methods like Paris' Law.

Simulation of fatigue damage in power semiconductors subjected to transient thermo-mechanical loading

Paul Hoffmann (*TU Wien, Austria*)

17:50

Martin Springer (*TU Wien, Austria*)

Melanie Todt (*TU Wien, Austria*)

Balamurugan Karunamurthy (*KAI - Kompetenzzentrum Automobil- u. Industrieelektronik GmbH, Austria, Infineon Technologies Austria AG, Austria*)

Michael Nelhiebel (*KAI - Kompetenzzentrum Automobil- u. Industrieelektronik GmbH, Austria, Infineon Technologies Austria AG, Austria*)

Heinz E. Pettermann (*TU Wien, Austria*)

Power semiconductors are often subjected to short electric overload pulses which induce very high temperature gradients in the metallization stack. Consequently, high mechanical stresses and strains occur, which in turn can lead to material failure. In preceding works [1,2] a continuum damage mechanics approach has been formulated and implemented into the finite element method which allows the prediction of damage onset and evolution of the material level as well as spatial damage evolution under cyclic thermo-mechanical loading conditions. Such a framework provides a step towards physical lifetime assessment of power semiconductor devices but, so far has only been used for quasi-static loading conditions.

As semiconductors are often subjected to transient thermal loads, the simulation framework is extended accordingly. The transient thermal and the mechanical fields are treated in a sequentially coupled manner. The time-dependent temperature field obtained from an initially conducted thermal analysis is used as input for the fatigue damage simulations. To account for the influence of the damage evolution on the local thermal conductivity, the transient temperature field is recomputed after a specific number of load cycles and the fatigue damage computations are resumed with the updated time-dependent temperature field.

The extended simulation methodology is applied to predict fatigue damage in the power-metallization layer of semiconductor devices. Realistic transient thermal boundary conditions are considered in the model. The simulation framework is formulated in a way that it can easily be adapted to different geometries and boundary conditions. One possible application for this framework would be the extraction of fatigue material parameters from experiments

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[2] G. Kravchenko, B. Karunamurthy, M. Nelhiebel, H. E. Pettermann: "Finite Element Analysis of Fatigue cracks Formation in Power Metallization of a Semiconductor Device Subjected to Active Cycling"; in: "Proceedings of the 14th Conference on Thermal, Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems", IEEE, Piscataway, NJ, (2013), Paper-Nr. 91, 6 S.

S03.03 | Damage and fracture mechanics

Date: February 20, 2019

08:30-09:30

Room: HS 50

Discretization approaches to model cutting mechanisms in single grit scratch processes with lagrangian, ALE and SPH formulations

Praveen Sridhar (*Technische Universität Kaiserslautern, Germany*)

08:30

Kristin de Payrebrune (*Technische Universität Kaiserslautern, Germany*)

Grinding is a manufacturing process with tightly bound geometrically indeterminate cutting edges. The geometrically indeterminate grits are formed by a plurality of bonded abrasive grits. They separate the material at high speed, with no permanent contact between the workpiece and the abrasive grain. The surface, shape and dimensional accuracy of a workpiece are changed to obtain a good surface finish. The institute of applied structural mechanics conducts experimental investigations and simulations to better understand the grinding process using the single grit approach. The material removal at an individual abrasive grit scale is composed of three phases rubbing, ploughing and cutting. The goal is to develop a physical force model of the grinding process, with which these process mechanisms can be predicted.

Despite of the significant technological progress in machining, at present it is very difficult to model cutting processes in order to predict optimal process performance. Lagrangian or eulerian finite element formulations are traditionally used to model the metal cutting process. A pure lagrangian approach is accurate with the representation of the domain boundary but requires a re-meshing procedure. A pure eulerian approach is used in order to compute a steady state solution, however its limitation lies in treatment of convective terms in the motion and constitutive equations. The Arbitrary Lagrange-Euler method (ALE) can be used to combine the advantages of both methods and avoid the disadvantages.

In context of the lagrangian simulation, use of a meshless technique, called SPH (Smooth Particle Hydrodynamics), has its advantage on large strain deformation problems without the need for re-meshing algorithms.

This work focuses on the comparison of the various discretization approaches for the cutting mechanism in a single grit scratch process and sheds much light on the advantages and disadvantages of each discretization approach.

Aspects of the particle finite element method applied to contact problems

Markus Schewe (*TU Dortmund, Germany*)

08:50

Andreas Menzel (*TU Dortmund, Germany, Lund University, Sweden*)

The Particle Finite Element Method (PFEM) developed by [1] is designed to allow changes in the outer shape of a body while performing a Finite Element Analysis. This is achieved by repeated remeshing and shape detection of a particle cloud, which represents the body under consideration. The shape detection method creates new surfaces if formerly connected points on the surface move away from each other sufficiently. This method allows to model material separation. Considering abrasive wear of surfaces, a mechanism-based approach aims to model such separation of surface particles on a mesoscale. The basis of this approach consists of a contact algorithm that captures the interaction of solid bodies. This contribution presents a contact domain method [2] which is implemented in PFEM. The approach uses the abilities of the shape detection method as a contact search method. The contact domains furthermore allow for non-matching surface grids. Numerical examples show the abilities of the approach in exemplary contact problems.

- [1] E. Onate, S. R. Idelsohn, F. Del Pin and R. Aubry. The Particle Finite Element Method. An Overview. *Int. J. Comput. Methods*, 1(2): 267-307 (2004).
- [2] J. Oliver, J.C. Cante, R. Weyler, C. Gonzalez and J. Hernandez. Particle Finite Element Methods in Solid Mechanics Problems. In: *Computational Plasticity. Computational Methods in Applied Sciences*, vol 7, edited by E. Onate and R. Owen (Springer, Dordrecht, 2007), pp. 87-103.

Numerical realization and fracture behavior of defect-free two-dimensional silica glass

Jan Stratmann (*RWTH Aachen University, Germany*)

09:10

Firaz Ebrahim (*RWTH Aachen University, Germany*)

Franz Bamer (*RWTH Aachen University, Germany*)

Bernd Markert (*RWTH Aachen University, Germany*)

The idea of the network structure of silica glass was already presented by Zachariassen in the early twentieth century [1]. An experimental verification was only published lately by introducing two dimensional silica glass on graphene [2]. The introduction of the new material offers a wide range of applications and helps to a further understanding of the mechanical behavior of amorphous and glassy materials. We present a new strategy that enables the numerical simulation of growing two-dimensional silica glass. In particular, a defect-free random network is produced geometrically. Within the framework of molecular dynamics, the network structure is minimized by means of the steepest descent method. A step-by-step extension of the network followed by energy minimization produces then the random, defect-free silica sample. The two-dimensional silica glass is subjected to tensile loading until the sample ruptures. We show that the material behavior differs significantly to the crystalline silica sample, which allows us to further understand the mechanical mechanism of plastification of amorphous and glassy materials.

[1] W.H. Zachariassen, *J. Am. Ceram. Soc.* 54 (1932) 3841.

[2] P.Y. Huang et al., *Nano Lett.* 12 (2012) 1081-1086.

S03.04 | Damage and fracture mechanics

Date: February 20, 2019

14:00-16:00

Room: HS 50

A gradient-plasticity approach to model the interaction between dislocation pile-up and cleavage initiation during fracture

Geralf Hütter (*TU Bergakademie Freiberg, Germany*)

14:00

Ngoc-Anh Giang (*TU Bergakademie Freiberg, Germany*)

Meinhard Kuna (*TU Bergakademie Freiberg, Germany*)

Many engineering metals like ferritic steels exhibit a transition from ductile fracture at room temperature or above to brittle fracture at low temperatures and/or increased rates of loading. The brittle behavior is associated with initiation and propagation of transgranular cleavage micro-cracks. These micro-cracks initiate from broken grain-boundary carbides, due to a dislocation pile-up at these sites.

In the present contribution, the complex interaction between dislocation-pile up at grain boundaries, cleavage initiation and ductile mechanism of failure is simulated. An efficient gradient plasticity model with micro-hard grain boundaries is used to model dislocation pile-up. Potential cleavage is modeled by a cohesive zone. Cell models are employed to address macroscopically uniform loading conditions. The simulation of initiation of crack growth requires to resolve discretely the micro-structure around a macroscopic crack tip in order to account for the highly

inhomogenous deformations in the fracture process zone. A parameter study exploits the sensitivity of the macroscopic fracture toughness on changes of microscopic parameters like strength of the constituents and grain size.

A gradient-extended damage-plasticity model for large deformations with nonlinear isotropic and kinematic hardening

Tim Brepols (*RWTH Aachen University, Germany*)

14:20

Stephan Wulfinghoff (*Kiel University (CAU), Germany*)

Stefanie Reese (*RWTH Aachen University, Germany*)

A gradient-extended damage-plasticity model for large deformations is presented that is based on a 'two-surface' methodology in which damage and plasticity are treated as distinct dissipative mechanisms by introducing separate yield and damage criteria as well as loading/unloading conditions (see e. g. [1]). The model accounts for both nonlinear isotropic and kinematic hardening and belongs to the class of micromorphic materials in the sense of Samuel Forest (see [2], [3]). It is able to cure the pathological mesh-dependence which is otherwise observable when using conventional 'local' models involving material softening. The theoretical framework of the model is discussed in detail and several numerical examples practically illustrate the model's mesh regularization properties in finite element simulations.

References:

- [1] T. Brepols, S. Wulfinghoff, and S. Reese, "Gradient-extended two-surface damage-plasticity: Micromorphic formulation and numerical aspects", *Int. J. Plast.* 97, 64-106 (2017)
- [2] S. Forest, "Micromorphic Approach for Gradient Elasticity, Viscoplasticity, and Damage", *J. Eng. Mech.* 135, 117-131 (2009)
- [3] S. Forest, "Nonlinear regularization operators as derived from the micromorphic approach to gradient elasticity, viscoplasticity and damage", *Proc. R. Soc. A* 472 (2016)

Numerical investigation of wear processes by a gradient-enhanced damage-plasticity model

Golnaz Hoormazdi (*Ruhr University Bochum, Germany*)

14:40

Klaus Hackl (*Ruhr University Bochum, Germany*)

Philipp Junker (*Ruhr University Bochum, Germany*)

The prediction of failure mechanism in structures are always an important topic in the field of computational mechanics. Finite element computations of an inelastic material involving softening behavior (e.g. softening plasticity or damage) can suffer from strongly mesh-dependent results. Therefore, such continuum models should be equipped with a regularization (localization limiter) strategy to overcome the above-mentioned problem.

In this study, we present a framework for gradient-enhancement for coupled damage-plasticity material model using the Hamilton's principle for non-conservative continua. This model shall be applied for the numerical investigation of wear processes as they occur, e.g. in the case of mechanized tunneling. These investigations require a fine resolution of the involved constituents (cut sheet and abrasive particles in the soil). Consequently, a modeling strategy for the damage-plasticity is needed for time-efficient simulations.

In this talk, we present a first step to the mentioned ultimate goal. To this end, a numerical framework for gradient-enhanced damage-plasticity coupling is proposed that is based on a combination of the finite element method with strategies from meshless methods. We demonstrate that this framework keeps the computational effort limited and close to the purely elastic problems. Several numerical examples prove the elimination of the pathological mesh dependency of results. Furthermore, first results to the simulation of wear in tunneling machines are presented.

Extended finite element method and gradient-enhanced damage model for a 3D dynamic crack problem under cyclical loading

Tengfei Lyu (*Leibniz Universität Hannover, Germany*)

15:00

Stefan Löhnert (*Technical University Dresden, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

The Extended finite element method (XFEM) is a special numerical method to handle arbitrary discontinuities in the displacement field independent of the finite element mesh. This is advantageous during crack initiation, growth and propagation processes. In the range of continuum damage mechanics, gradient-enhanced damage models [1] can be used to model damage and fracture without spurious mesh dependencies. Gradient-enhanced damage models have been investigated extensively in the context of quasi-brittle and elasto-plastic materials.

To avoid fracture and failure of metallic materials in industrial engineering, modelling the component under cyclical loading is significant for fatigue life-time prediction [2]. Fatigue damage increases in a cumulative manner, along with the number of applied loading/displacement cycles, resulting in crack formation and final failure of the component.

In this paper, a 3d dynamic crack problem under cyclical loading is studied on a mesoscale. Finite deformation elastoplasticity is coupled with gradient-enhanced damage. The domain is discretized with 2nd-order ten-node tetrahedral elements. Discrete cracks are captured using the XFEM. The crack geometry is updated by level set methods. The focus of this contribution is set on algorithmic issues.

References:

- [1]. Peerlings, R.H.J., De Borst, R., Brekelmans, W.A.M., De Vree, J.H.P.: Gradient enhanced damage for quasi-brittle materials. *Int. J. Numer. Methods Eng.* 39(19), (1996), pp.3391-3403
- [2]. E. Santecchia, A. M. S. Hamouda, F. Musharavati, et al., A Review on Fatigue Life Prediction Methods for Metals, *Advances in Materials Science and Engineering*, vol. (2016), 26 pages.

On the energetics of dynamic cohesive crack formation

Tobias Laschütza (*Karlsruhe Institute of Technology (KIT), Germany*)

15:20

Thomas Seelig (*Karlsruhe Institute of Technology (KIT), Germany*)

Owing the Griffith's criterion, brittle fracture takes place once the released energy equals the required fracture surface energy. However, in case of the spontaneous formation of a finite crack, as considered e.g. in the framework of finite fracture mechanics [1], a certain amount of the released energy is converted into kinetic energy during the fracture process. Thus, this portion of energy is not available to overcome the fracture energy.

In the present work, the different energy portions involved in the spontaneous (dynamic) formation of cracks in statically pre-stressed bodies is analysed from 1D and 2D examples. In the 1D case of a tensile bar undergoing cohesive fracture, it turns out that the kinetic energy at the instant of complete fracture equals about 50 % of the fracture energy. That is, in this case the necessary released energy has to be 50 % higher than the fracture energy in order to cause complete fracture.

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S03.05 | Damage and fracture mechanics

Date: February 20, 2019

16:30-18:30

Room: HS 50

Identifying the non-local interactions of self-adhesive polymeric films with digital images of T-peeling

Behnaz Bagheri (*Otto-von-Guericke-Universität, Germany*)

16:30

Konstantin Naumenko (*Otto-von-Guericke-Universität, Germany*)

Holm Altenbach (*Otto-von-Guericke-Universität, Germany*)

Flexible polymer films with self-adhesive properties are widely used in different fields because of their modifiable properties. Even the poor surface adhesion of such films can be improved with surface modification methods such as cling layer co-extrusion (which can provide the self-adhesive properties for the film). To analyze and determine the delamination behaviour of such films, the interaction forces between the surfaces are required. The interactions between such self-adhesive polymeric films are from the Van der Waals type.

In this contribution, a new feature of non-local interactions was taken into account for modeling the adhesive forces of thin polymeric films with self-adhesion. The idea is to identify these interactions from digital images of the deformed flexible films during the film delamination under T-peel test. However, the performance of the model can be checked by other popular peel tests. The images of the deformed shape of the films and the measured peel forces were the output data of the experiments. According to these images, which were taken perpendicular to the transverse view, the curvature shape of the films during the peel test can be calculated and inserted into the model for further analyzations to identify the properties of the adhesive layer.

J-integral and cohesive zones of mixed-mode interface and matrix cracks

Johannes Scheel (*Universität Kassel, Germany*)

16:50

Andreas Ricoeur (*Universität Kassel, Germany*)

In 1968 Rice introduced the J-integral [1] which turned out to be a powerful and accurate tool for calculating crack tip loadings. The extended formulation by Budiansky and Rice [2] also enables the calculation of crack deflection angles using the J-integral criterion. It can not only be used to calculate matrix crack tip loadings but interface crack tip loadings as well. At the beginning limited to J_I [3], an extension also considered the second coordinate for interface cracks [4]. For a pure mode I case, Rice related the J-integral to the crack tip opening displacement as crack tip loading quantity of cohesive zone models. A generalization to that relation is formulated and verified in this work, accounting for mixed mode loading conditions. This extension also enables the formulation of a criterion for the transition of an interface crack to a matrix crack, whereat the J-integral criterion needs a modification.

The interaction between a matrix and an interface crack is investigated too. Calculating the matrix crack tip loading in the presence of an interface crack using remote integration contours reveals, that the interface crack tip loading is included therein.

[1] Rice, J. R.; Journal of Applied Mechanics 1968; 35: 379-386.

[2] Budiansky, B., Rice, J.R.; Journal of Applied Mechanics 1973; 40: 201-203.

[3] Smelser, R. E., Gurtin, M. E.; International Journal of Fracture 1977; 13: 382-384.

[4] Khandelwal, R., Kishen, C. J. M.; Engineering Fracture Mechanics 2006; 73: 1568-1580.

A finite fracture mechanics approach for interlaminar crack initiation using the scaled boundary finite element method

Sebastian Dölling (*TU Darmstadt, Germany*)

17:10

Sophia Bremm (*TU Darmstadt, Germany*)

Sascha Hell (*TU Darmstadt, Germany*)

Wilfried Becker (*TU Darmstadt, Germany*)

Highly localised interlaminar stresses arise at free edges of composite laminates. These stresses are induced by layer-wise different stiffness properties and have been investigated by Pipes and Pagano [1]. The question arises whether interlaminar stresses may yield premature failure by interlaminar crack onset. Common strength based criteria are unsuitable due to the theoretically infinite stresses at the free edge. Energy based fracture mechanics approaches are restricted to pre-existing cracks and hence not adequate. To surpass these limitations, Hashin [2] proposed the instantaneous formation of cracks of finite size, leading to the finite fracture mechanics approach (FFM). However, the finite crack size must be determined additionally. Thus, Leguillon [3] suggested a coupled stress and energy criterion to identify the unknown failure load as well as the corresponding finite crack size. Based on the coupled criterion, Martin et al. [4] examined interlaminar crack onset in symmetric angle-ply laminates, whereby the required quantities were determined using a finite element model.

In the present study, interlaminar crack initiation, induced by the free-edge effect, is investigated using the coupled stress and energy criterion. For that purpose, the underlying mechanical model corresponds to the Pipes and Pagano model. The semi-analytical scaled boundary finite element method (SBFEM), introduced by Song and Wolf [5], is used in order to significantly reduce computational effort. Only the boundary is discretized by finite elements whereas the solution in the interior body is represented analytically by solving an ordinary differential equations system. Furthermore, the SBFEM allows access to the weighted deformation modes. The obtained field quantities are in agreement to a classical finite element reference solution. The predicted resistance to interlaminar crack initiation is compared to experiments from literature.

[1] R.B. Pipes and N.J. Pagano. Interlaminar stresses in composite laminates under uniform axial extension. *Journal of Composite Materials*, 4:538-548, 1970.

[2] Z. Hashin. Finite thermoelastic fracture criterion with application to laminate cracking analysis.

Journal of the Mechanics and Physics of Solids, 44(7):1129-1145, 1996.

[3] D. Leguillon. Strength or toughness? A criterion for crack onset at a notch. *European Journal of Mechanics-A/Solids*, 21(1):61-72, 2002.

[4] E. Martin, D. Leguillon, N. Carrere. A twofold strength and toughness criterion for the onset of free-edge shear delamination in angle-ply laminates. *International Journal of Solids and Structures*, 47:1297-1305, 2010.

[5] C. Song and J.P. Wolf. The scaled boundary finite-element method - alias consistent infinitesimal finite-element cell method for elastodynamics. *Computer Methods in Applied Mechanics and Engineering*, 147:329-355, 1996.

Implementation of generalized mechanical interfaces

Lucie Spannraft (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

17:30

Julia Mergheim (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

Paul Steinmann (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

For an accurate approximation of the mechanical behavior of interfaces undergoing tensile, shear and stretch deformation, the definition of an appropriate interface constitutive model is crucial. Cohesive zone models (CZM) are generally formulated to describe the geometrically non-coherent non-energetic interface response to tensile and shear loading. CZM are well investigated and distinct cohesive laws can be implemented by means of various options i.a. in commercial FEM software, such as ABAQUS. A limitation of CZM interfaces is the lack of any energetic structure along the interface. Thus, the cohesive interface allows for displacement jumps, but no traction jumps, i.e. no in-plane stretch. For this reason, an extension of the CZM to a generalized mechanical interface model is required. Combining the CZM with interface inelasticity allows performing valid numerical simulations of non-coherent energetic interfaces. Although interface elasticity is widely discussed in the literature, only little research considering interface inelasticity and generalized mechanical interfaces is conducted, for instance refer to [2, 3]. Furthermore, to the authors' knowledge no incorporation of such a model in ABAQUS is available. In order to benefit from the advantages of commercial software, this contribution presents an approach to implement large-deformation generalized mechanical interfaces in the commercial FEM software ABAQUS: Zero thickness user elements, which may have a curved smooth or a non-smooth geometry, are generated at the interface in ABAQUS. A user subroutine solves the element stiffness matrix and force vector for each user element. As constitutive model of the interface, a damage-type traction-separation law with exponential softening according to [4] and an interface hyperelasticity model accounting for in-plane degradation based on [1, 2] are coupled by their damage variables, compare [2].

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[2] A. Esmaceli, A. Javili, P. Steinmann. Non-coherent energetic interfaces accounting for degradation. *Comput Mech*, 59(3), 361-383 (2017)

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An interface model to account for damage and plasticity at grain boundaries

Shahed Rezaei (*RWTH-Aachen University, Germany*)

17:50

Jaber Rezaei Mianroodi (*RWTH-Aachen University, Germany, Max-Planck-Institut für Eisenforschung GmbH, Germany*)

Tim Brepols (*RWTH-Aachen University, Germany*)

Stephan Wulfinghoff (*Christian-Albrechts-Universität zu Kiel, Germany*)

Stefanie Reese (*RWTH-Aachen University, Germany*)

Grain boundary (GB) characteristics play a major role in the understanding and prediction of polycrystalline behavior. GB roles becomes more important when it comes to nanocrystalline metals and ceramics. To gain a deeper insight into the behavior of the grain boundary, molecular dynamics (MD) simulations are utilized. The Mode I, mode II and mixed mode loading behavior is investigated using different MD simulations. By adding the unloading path to the MD simulations it was possible to differentiate between different active mechanisms at the GB. An interface model is introduced based on our understanding from atomistic simulation of the grain boundaries. When it comes to the grain boundary (GB) behavior, current model is able to capture the competition between the intergranular fracture and the grain boundary sliding. The interface model is thermodynamically consistent and is able to capture the complex behavior of the GB under different loading conditions.

S03.06 | Damage and fracture mechanics

Date: February 21, 2019

08:30-10:30

Room: HS 50

A computational framework for brittle crack-propagation based on efficient virtual element method

Ali Hussein (*Leibniz Universität Hannover, Germany*)

08:30

Fadi Aldakheel (*Leibniz Universität Hannover, Germany*)

Blaž Hudobivnik (*Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

Pierre-Alain Guidault (*LMT, ENS Paris-Saclay/CNRS/Université Paris-Saclay, France*)

Olivier Allix (*LMT, ENS Paris-Saclay/CNRS/Université Paris-Saclay, France*)

An efficient low order virtual element method (VEM) for crack-propagation in elastic solids at small strains is outlined within this work. The recently developed VEM is a competitive discretization scheme for meshes with highly irregular shaped elements and arbitrary number of nodes [1]. The formulation in this contribution is based on minimization of an energy expression with stabilization techniques for brittle fracture in 2D problems [2, 3]. Novel aspect here is the development of robust cutting techniques through elements for crack propagation in two-dimensional solids using VEM. The performance of the formulation is underlined by means of representative examples.

References:

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- [3] P. Wriggers, B. D. Reddy, W. Rust, and B. Hudobivnik. Efficient virtual element formulations for compressible and incompressible finite deformations. *Computational Mechanics*, 60(2):253-268, 2017.

Crack paths in ferroelectrics: crack growth simulation and experiments

Zhibin Wang (*University Kassel, Germany*)

08:50

Andreas Ricoeur (*University Kassel, Germany*)

Ferroelectric materials are in widespread use as smart materials in many industrial applications, e.g. as sensors or actuators. An important prerequisite of utilization of such materials is a fundamental understanding of the general cracking behaviour, especially their behaviour under electric field and how the ferroelectric effect affects the crack path. Many researchers have been working on this topic for years [1]. However, some issues are still not understood.

In this work theoretical analyses and experimental observations of crack growth and deflection in ferroelectric materials are presented. The application of a generalized energy release rate, which is divided into mechanical and electrical parts, is discussed with respect to fracture threshold and crack deflection. Classical crack deflection criteria are adjusted due to specific properties of ferroelectrics. The anisotropy of the crack resistance parameters turns out to play a crucial role

in the crack deflection. A re-meshing algorithm in connection with a FE-code is used to simulate crack paths under diverse mechanical-electric loading combinations. A three point bending test set-up is further presented based on previous work [2] and some results are shown.

[1] T.Y. Zhang, C.F. Gao. Fracture behaviors of piezoelectric materials. *Theor. Appl. Fract. Mec.* 41, (2004), 339 -379.

[2] S. Park, C. Sun. Fracture criteria for piezoelectric ceramics. *J. Am. Ceram. Soc.* 78(6), (1995), 1475-1480.

Micromechanical simulation of crack growth resistance curve in ferroelectrics

Meinhard Kuna (*TU Bergakademie Freiberg, Germany*)

09:10

Sergii Kozinov (*TU Bergakademie Freiberg, Germany*)

In ferroelectric ceramics, switching of domains leads to a change of both polarization and remanent strains. This affects substantially the stress state and electric field in the vicinity of a crack tip and the fracture behavior. While domain switching around stationary cracks has been analyzed quite well, the focus of the present work lies on the evolution of domain pattern during slow crack growth.

The domain switching processes are simulated by a 3D micromechanical constitutive model. Crack growth is numerically realized by means of electromechanical cohesive elements along the prospective crack path. Both models are implemented in the finite element code Abaqus.

In particular, the spatial distribution of domain orientations in a mechanically loaded CT-specimen of PZT-PIC151 ceramic is computed and compared with in-situ X-ray diffraction experiments in synchrotron. It is found that the preferred orientation and intensity of domain distribution around the crack tip agree well with experimental observations, and are related to the deviatoric stresses/strains. During crack propagation, the maximal tensile stresses and region of highest intensity of domain reorientation are moving with the crack tip and smeared over a process zone. Hereby, the domain switching zone causes a shielding effect, which leads to a rising fracture resistance curve and an apparent materials toughening.

Mixed-mode fracture: the missing link between J-vector criterion and conventional fracture criteria

Paul Judt (*University of Kassel, Germany*)

09:30

Andreas Ricoeur (*University of Kassel, Germany*)

In the past decades different crack growth and crack deflection criteria have been proposed, e.g. the maximum hoop stress criterion [1], the minimum strain energy density criterion [2] or the maximum energy release rate criterion [3]. These criteria were extended concerning phenomena such as crack path instability [4,5] and the anisotropy of fracture parameters [4]. Another approach for the prediction of crack growth and deflection angle is based on the J_K -integral assuming the crack to grow into the direction of the J -vector. The resulting deflection angles coincide well with other criteria in the case of small mixed-mode ratios K_{II}/K_I . One challenge is the accurate calculation of the second coordinate J_2 [6] and the appropriateness of this approach has been shown [7]. Nevertheless, in the case of anisotropic crack resistance parameters, large mode-II loadings or instable crack paths, the J -vector criterion fails.

An effective J -vector J_k^{eff} is introduced providing the correct crack growth direction in the cases of anisotropic fracture parameters [7,8], arbitrary mixed-mode loadings and crack path instabilities. The effective J -vector accounts for an orientation dependent crack resistance parameter $J_c(\phi)$ as well as for contributions of material forces on crack faces in the vicinity of the crack tip due to a mode-II loading and the T -stress. The theory is validated by experimental results and applied to numerical crack path predictions.

References

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- [8] P.O. Judt, J.C. Zarges, A. Ricoeur, H.P. Heim, Anisotropic fracture properties and crack path prediction in glass and cellulose fiber reinforced composites. *Engineering Fracture Mechanics*, 188:344-360, 2018.

Scaled boundary finite element I modelling of thermally induced crack propagation

Muhammad Danish Iqbal (*Universität Duisburg-Essen, Germany*)

09:50

Carolin Birk (*Universität Duisburg-Essen, Germany*)

Thermal shock is a phenomenon that often occurs in high temperature processes. It is associated with rapid temperature changes and very high temperature gradients, which cause thermal stresses. These thermal stresses can produce fracture and damage in brittle materials such as ceramics. The modelling of such processes is a very challenging task due to the rapid development of complex crack networks.

The simulation of discrete crack propagation processes requires numerical methods that can represent stress singularities accurately and efficiently. In the context of linear elastic fracture mechanics, the scaled boundary finite element method (SBFEM) has gained popularity. One of the main features of this semi-analytical method is the ability to model stress singularities present at the crack tips very effectively and accurately. The SBFEM combines a numerical solution in the circumferential directions with an analytical solution in the radial direction of the considered domain. It also facilitates the derivation of generalized polygon elements and thus provides great flexibility in the meshing of complex geometries. In crack propagation modelling, such elements require minimal re-meshing in the vicinity of the crack tip.

The principles of the scaled boundary finite element method for transient thermal analysis and for thermal stress analysis will be summarized in this contribution. Various examples will be presented to illustrate the potential of the SBFEM in the context of thermally induced crack propagation modelling.

Crack propagation using incompatible modes in structural elements

Andjelka Stanic (*Technische Universität Braunschweig, Germany*)

10:10

Bostjan Brank (*University of Ljubljana, Slovenia*)

Adnan Ibrahimbegovic (*Université de Technologie de Compiègne – Sorbonne Universités, France*)

In order to describe a crack formation and opening in quasi brittle 2d solids we use the method of embedded strong discontinuity in displacements that provides mesh-independent solution. Namely, the fracture dissipation energy is associated with the discontinuity and does not depend on the finite element size. Crack opening is expressed as a combination of basic separation modes (mode I and mode II). The cohesion tractions in the crack are described by damage-softening constitutive relation. We derived a novel quadrilateral finite element with embedded strong discontinuity that is improved by incompatible mode parameters. Several quadrilateral formulations related to the plane stress finite element with embedded strong discontinuity in displacements are studied. Results of a set of numerical examples are provided in order to assess the performance of the novel embedded strong discontinuity quadrilateral finite element formulation and the crack tracing algorithm.

S03.07 | Damage and fracture mechanics

Date: February 21, 2019

14:00-16:00

Room: HS 50

Mechanical microstructure characterization of discontinuous-fiber reinforced composites by means of experimental-numerical micro tensile tests

Michael Schober (*Fraunhofer Institute for Mechanics of Materials IWM, Germany, Karlsruhe Institute of Technology (KIT), Germany*)

14:00

Kerstin Dittmann (*Fraunhofer Institute for Mechanics of Materials IWM, Germany*)

Peter Gumbsch (*Karlsruhe Institute of Technology (KIT), Germany*)

Takashi Kuboki (*University of Western Ontario, Canada*)

Jörg Hohe (*Fraunhofer Institute for Mechanics of Materials IWM, Germany*)

The mechanical characteristics and especially the damage behavior of discontinuous-fiber reinforced composites greatly depend on its constituents and also on its microstructural properties, namely the extent and distribution of fiber agglomerations, the fiber orientation distribution, and the fiber-matrix interfaces. Several methods exist to individually analyze the different microstructural properties, such as μ CT scanning to obtain the distribution of the fibers and their orientation and the Microbond test to obtain the interfacial characteristics. However, the interdependencies of the individual characteristics and the initiation of fracture with respect to the microstructure are still hard to analyze regarding a real composite structure. For this reason, the microscopic fracture behavior of a glass fiber reinforced sheet molding compound (SMC) shall be investigated by means of a micro tensile test. Therefore, a specimen with a gauge length of approx. 1 mm, 0.3 mm width and 0.1 mm thickness is extracted from a composite plaque and put to an in-situ observed tensile test. With a finite element model of each specimen, including the position and orientation of each fiber, the fiber-matrix-interface characteristics are extracted with a reverse-engineering approach. The tests show a microstructure-specific fracture behavior, which depends on the fiber dispersion, the fiber orientation, and the fiber-matrix interfaces. The numerical simulations well agree with the physical experiments, making the obtained parameters suitable for further simulations of the investigated structure on a larger scale.

Numerical analysis of the thermally induced damage in remote laser cut carbon fiber reinforced polymers

Benjamin Schmidt (*TU Dresden, Germany*)

14:20

Michael Rose (*TU Dresden, Germany*)

Martina Zimmermann (*TU Dresden, Germany*)

Markus Kästner (*TU Dresden, Germany*)

In cutting technologies for fiber reinforced polymers, remote laser cutting plays a special role because it can minimize the drawbacks of other laser cutting methods, e.g. frayed cutting edges, caused by the high heat input of the laser. It allows precise cutting results even for high spot velocities and sharp edges, which facilitates a reduction of the heat input and thus decreased thermal damages. For a reliable structural analysis, it is necessary to quantify these damages and its possible effects on static and fatigue failure have to be determined.

In this contribution the Pinho material model is used to describe the static damage behavior. Compared to simpler failure models, this material model is characterized by a physically based failure criterion for the different damage modes. In the first part of this presentation, the parametrization of the material model is outlined, whereat the focus is on tensile and shear failure modes. In order to determine stiffness and strength, tensile tests were performed and used for the validation of the simulationmodel.

In the second part of this contribution, a model to describe and analyse thermal damage caused by laser cutting is presented. The dimensions of the damaged area are taken from polished micro sections of the material around the edge. The spatial distribution of the damage in the specimen depends on the temperature field caused by the laser and is described as a function of the distance between a material point and the laser cutting edge. These predefined damages are modelled with the damage parameters of the static damage model, which allows a mapping of the damaging effects to the damage modes and a separated modelling of the different effects. As an example, comparative tensile tests of water jet and laser cut open hole specimens are simulated. The advantage of these specimen is the predefined localization of damage at the cutting edge of the holes, which allows a direct comparison of the cutting technologies due to the controlled heat input at the failure area around the hole.

Development and validation of a virtual process chain for sheet molding compound composites

Johannes Görthofer (<i>Karlsruhe Institute of Technology, Germany</i>)	14:40
Nils Meyer (<i>Karlsruhe Institute of Technology, Germany</i>)	
Ludwig Schöttl (<i>Karlsruhe Institute of Technology, Germany</i>)	
Anna Trauth (<i>Karlsruhe Institute of Technology, Germany</i>)	
Malte Schemmann (<i>Karlsruhe Institute of Technology, Germany</i>)	
Pascal Pinter (<i>Karlsruhe Institute of Technology, Germany</i>)	
Martin Hohberg (<i>Karlsruhe Institute of Technology, Germany</i>)	
Tarkes Dora Pallicity (<i>Karlsruhe Institute of Technology, Germany</i>)	
Kay A. Weidenmann (<i>Karlsruhe Institute of Technology, Germany</i>)	
Peter Elsner (<i>Karlsruhe Institute of Technology, Germany</i>)	
Frank Henning (<i>Karlsruhe Institute of Technology, Germany</i>)	
Andrew Hrymak (<i>University of Western Ontario, Canada</i>)	
Thomas Seelig (<i>Karlsruhe Institute of Technology, Germany</i>)	
Luise Kärger (<i>Karlsruhe Institute of Technology, Germany</i>)	
Thomas Böhlke (<i>Karlsruhe Institute of Technology, Germany</i>)	

Sheet Molding Compound (SMC) composites are of great interest in industry sectors (e.g., automotive, aerospace and sports) as the production cycles are short and cost efficient. They are suitable for mass-reduction strategies due to their high mass-specific strength and stiffness relative to other classes of composites. A profound understanding of the material behavior and the influences of the production process are crucial for structural applications of SMC composites. However, the design and optimization of a specific component using conventional trial-and-error methods within a physical process chain are quite time-consuming and expensive. These problems can be circumvented via a robust and accurate virtual process chain.

Within this work, the physical process chain of a defined SMC composite demonstrator part is presented. A corresponding virtual process chain (consisting of the key steps compression molding and structural simulation) is established and validated by means of experimental investigations. The compression molding is simulated via a Coupled-Eulerian-Lagrangian approach due to the significant flow of the material during the process. The SMC is modeled as an anisotropic Newtonian fluid during the flow phase. The evolution of the fiber orientation distribution (FOD) is described by Jeffrey's equation including an invariant-based optimal fitting closure for the fourth-order fiber orientation tensor (FOT). The simulated FOD at the end of the compression molding is validated by means of experimental measurements carried out via computed tomography (CT) scanning of the fabricated demonstrator. The predicted FOD is seamlessly transferred by mapping the data from an Eulerian mesh onto a structural mesh using a neutral visualization toolkit (VTK) data format. Based on the FOD data, structural simulations are carried out using a mean-field anisotropic damage model to predict the damage evolution in the demonstrator. The model captures the dominant damage mechanisms in SMC composites, namely matrix cracking and fiber-matrix interface debonding. A consistency condition based on a statistical Weibull approach for the interface strength ensures a proper anisotropic and inhomogeneous reduction of the load-carrying fiber fraction.

The structural simulations are validated by means of a four-point bending test on the demonstrator (static and cyclic). Hereby experimental observations are compared to structural simulation results with FOD input coming from measured CT scans and from compression molding simulations. Additionally, the influence of different fiber orientation states of the demonstrator part is investigated. The predicted results of each step of the virtual process chain indicate satisfying accuracy.

Development of a novel damage approach on the microstructure for modelling woven Ceramic Matrix Composites

Marie-Christine Reuvers (*RWTH Aachen University, Germany*)

15:00

Shahed Rezaei (*RWTH Aachen University, Germany*)

Tim Brepols (*RWTH Aachen University, Germany*)

Stefanie Reese (*RWTH Aachen University, Germany*)

Ceramic Matrix Composites (CMC) overcome limitations associated with classical technical ceramics e.g. low fracture toughness and brittle failure under mechanical or thermomechanical loading (e.g., Chawla., 2013). Their high temperature stability and low weight makes them attractive for use in various fields, especially aerospace industry, where they improve engine efficiency compared to metal components. However current CMCs lack well established material property design databases for a reliable use in critical aerospace structures. Demonstrating the durability of this relatively new class of materials is the challenge to face and therefore the failure mechanisms need to be investigated further. This contribution deals with the successive development of a woven representative volume element (RVE) for arbitrary CMCs. In contrast to previously developed continuum mechanical or laminate theory based modeling approaches, the introduced model combines various damage formulations. The fiber bridging effect, resulting from the weak interface bond of matrix and reinforcement, is governed by the use of cohesive zone (CZ) elements (e.g., Rezaei et al., 2017). Whereas the matrix damage is represented using a continuum mechanical approach (e.g., Brepols et al., 2017). To cover temperature effects, thermal coupling will be included in both element formulations in future works.

Chawla, K.K., Ceramic Matrix Composites. Springer Science & Business Media.

Rezaei, S., Wulfinghoff, S., Reese, S., 2017. Prediction of fracture and damage in micro/nano coating systems using cohesive zone elements. International Journal of Solids and Structures 121, 62-74.

Brepols, T., Wulfinghoff, S., Reese, S., 2017. Gradient-extended two-surface damage-plasticity: micromorphic formulation and numerical aspects. *International Journal of Plasticity* 97, 64-106.

Verification and validation of a 2D energy based peridynamic state-based failure criterion

Christian Willberg (*German Aerospace Center, Germany*)

15:20

Martin Rädcl (*German Aerospace Center, Germany*)

Heinecke Falk (*German Aerospace Center, Germany*)

The paper presents a verification and validation approach for peridynamic failure models. The use-case at hand is an enhanced energy-based failure model for state-based peridynamics. Solution robustness and validity of predicted crack initiation and propagation is demonstrated for a double cantilever beam.

Tensile tests using the same material and energy release rate from the prior simulations are used to predict specimen failure. The model is implemented in the software Peridigm and will be published open-source.

Computationally effective spot-weld fatigue life estimation for vehicle components

Milan Zigo (*MAGNA STEYR Engineering, Austria*)

15:40

Eray Arslan (*TU Wien, Austria*)

Werner Mack (*TU Wien, Austria*)

Gerhard Kepplinger (*MAGNA STEYR Engineering, Austria*)

Fatigue in vehicle components is caused by various excitations within a broad frequency-range and is an important issue in automotive industry. However, in spite of the high performance of present-day computers, FE fatigue analyses in the time-domain for complex models with huge degrees of freedom still are very time consuming. Hence, frequency-domain methods find more and more application at early stages of the design process. Whereas in general these methods are well-established, there still is room for improvements in their application to special problems. For example, this applies to components with many spot-welds (about 4000-6000 in a typical body-in-white of a modern vehicle). Essentially, in time-domain analyses of spot-weld fatigue two basic approaches have been followed: First, there are simple FE-models with only a few elements which allow for a rather gross approximation of the stress state only. Second, there are detailed models with hundreds or thousands of nodes for a single spot-weld, which however are computationally very expensive. Whereas this is a crucial issue especially in time-domain calculations, improvements in frequency-domain procedures for components with a large number of spot-welds are possible, too.

Hence, the present contribution suggests an algorithm with several measures to speed up the computations in the frequency-domain further. For example, first in a modal analysis of the entire structure a rather coarse mesh is applied. Then, the grid point forces at the spot-welds are appropriately transformed to inputs for spot-weld models with fine mesh out of a pre-processed library. These models are available for many different spot-weld- and sheet-geometries and unit load cases. The real notch stresses then are obtained as a superposition of normal stress over all modes with consideration of the transfer function (from a frequency response analysis) and multiplication with given input PSD. Moreover, the so-called cutting-plane method is used, and based thereon efficient a priori stress estimates are implemented to reduce the grid points to be considered further in Dirlik's method to obtain the PDF of occurring stress ranges and subsequently the fatigue life. Thus, the fatigue effects of qualitatively and quantitatively different

load histories may be investigated with high reliability within short time, and this is illustrated by examples of actual vehicle components.

S03.08 | Damage and fracture mechanics

Date: February 22, 2019

08:30-10:30

Room: HS 50

Detection of cracks and notches based on the monitoring of remote strain fields and the distributed dislocation technique

Ramdane Boukellif (*University of Kassel, Germany*)

08:30

Andreas Ricoeur (*University of Kassel, Germany*)

Engineering structures are in general exposed to cyclic or stochastic mechanical loading. Exhibiting incipient cracks, particularly light-weight shell and plate structures suffer from fatigue crack growth, limiting the life time of the structure and supplying the risk of a fatal failure. Due to the uncertainty of loading boundary conditions and the geometrical complexity of many engineering structures, numerical predictions of fatigue crack growth rates and residual strength are not reliable. Most experimental monitoring techniques, nowadays, are based on the principle of wave scattering at the free surfaces of cracks. Many of them are working well, supplying information about the position of cracks. One disadvantage is that those methods do not provide any information on the loading of the crack tip. In this work, the development of a concept for the detection of cracks and notches in finite plate structures under mixed mode loading conditions is presented. In this approach, the distributed dislocation technique is applied to model the direct problem and a genetic algorithm is used to solve the inverse problem. As an approach, different from the FEM, cracks are modelled with a collocation of discrete dislocations. Thus, it is not necessary to discretize the domain around the crack, considerably saving computation time and data, which is crucial for an efficient solution of the inverse problem. Solving the inverse problem, e.g. with a genetic algorithm this allows the identification of external loading, crack or notch position parameters, such as length, location or angles, and the calculation of stress intensity factors. Experiments are performed using plates with notches under tensile loading.

Noise reduction for DIC measurements and single strut testing

Martin Reis (*Saarland University, Germany*)

08:50

Stefan Diebels (*Saarland University, Germany*)

Anne Jung (*Saarland University, Germany*)

Digital image correlation (DIC) is well known as a contactless measuring method to evaluate strain and displacement fields on the specimen surface. Due to the low needs on the setup and relatively easy specimen preparation, the usage is widely spread for full-field strain and displacement measurements. Nevertheless, there are error sources such as light settings, spackle pattern and noisy images, which often stay uninvestigated. Therefore, this work displays a simple routine, which allows to identify the error in the images and enhance the DIC accuracy. A calibration sample adapted to the specifications of the setup use the beam theory to link machine displacement, DIC measurements and the forces. The evaluation is done in the commercial software ISTR4D®. The noise in the measurements is reduced to an error of under two percent. The routine allows to estimate the quality of the images before performing the experiments. Furthermore, the routine is transferable to all experimental setups. The calibration of the setup allows to get reliable experimental results with a known error. With this estimated stochastic error, the advantages of DIC can be used to evaluate mechanical experiments. One example is

the investigation of hybrid foams, such as a polyurethane (PU) foam coated with nanocrystalline nickel (Ni). This material has a high energy absorption capacity and a low price. The combination promises good applicability as a crash absorber. To achieve this, experiments must be carried out on single pores and struts. Due to the complex structure of the foam and individual struts, only a contactless strain measurement, such as DIC is possible. Three-point bending and tensile tests on single struts demonstrate the quality of the setup. For both experiment types a rise of the local strain, before a visible crack appears, as well as the real total strain can be measured. This work presents a routine, which helps to estimate and reduce the error of the DIC measurements and gives a proof of principle of the method with experiments on single struts of a Ni/PU hybrid foam. Which is important for the conclusive modelling of the material.

Investigations on biaxial specimens for anisotropic damage evolution in SMC

Juliane Lang (*Karlsruhe Institute of Technology KIT, Germany*)

09:10

Malte Schemmann (*Karlsruhe Institute of Technology KIT, Germany*)

Thomas Seelig (*Karlsruhe Institute of Technology KIT, Germany*)

Thomas Böhlke (*Karlsruhe Institute of Technology KIT, Germany*)

Sheet moulding compound (SMC) as a discontinuous fiber reinforced composite combines high strength and stiffness and a low density with an economical production and is, thus, an ideal lightweight material. The detailed understanding of the mechanical behavior of SMC presents, however, a challenge to composite material science.

Biaxial tensile tests allow the investigation of damage evolution under multiaxial stress states, which is particularly interesting due to the different damage phenomena in composite materials. A key challenge is to find a suitable specimen shape, because typical cruciform specimens fail in the arms before damage occurs in the area of interest which is the area of the biaxial stress state in the center area of the specimen. In preliminary investigations suitable specimen designs were developed and compared with regard to different criteria, especially, with regard to the maximum reached strain in the center area before failure. For all introduced designs and for a uniaxial bone specimen for comparison the stiffness degradation as one phenomenon of damage is analyzed and compared as a further optimality investigation. For the best performing specimen which is reinforced by unidirectional reinforced tapes on the arms, further investigations are performed. The strain field, especially, in the center area and at critical points is analyzed by finite element simulations. For the investigation of anisotropic damage evolution biaxial tensile tests with different loading ratios are performed and evaluated with respect to stiffness reduction. The results of these investigations can be used to perform an inverse parameter identification and to validate mean field homogenization approaches of the elastic properties and, especially, anisotropic damage models. Micro computed tomography scans can deliver the data for the microstructure-based models.

Simulation of subcritical crack propagation in hard metal microstructures

Dennis Wingender (*Ruhr-University Bochum, Germany*)

09:30

Daniel Balzani (*Ruhr-University Bochum, Germany*)

The efficient operation of mechanized tunnel drilling machines is strongly determined by the wear resistance of the applied mining tools. Especially in chisels, but also partly in cutting disks, hard metals are used. Their wear mechanism is dominated by surface spalling, i.e. subcritical crack propagation through the material's microstructure mainly consisting of a ductile metal matrix and carbide inclusions. Since this process is mainly governed by the morphology of the microstructure and the mechanical behavior of the individual phases, simulations at the microscale enable the design of improved materials. In this contribution a method for the modeling of this

process is presented. The approach is based on the eigen-erosion framework introduced in [1] and an algorithmic scheme for large strains is given, which extends the small strain implementation in [2]. For the phases at the microscale the finite strain plasticity formulation [3] is applied and parameters are chosen in line with experimental data. In order to keep the computational effort moderate the concept of statistically similar RVEs [4] is used. Thereby, artificial microstructures with a significantly reduced complexity and thereby less finite elements are considered which still represent the morphology statistics as good as possible. Representative numerical examples are given to show the performance of the method. In these simulations where cyclic loading below the yield strength is applied the crack grows with increasing cycle number due to plastic flow and the change of the loading paths caused by the previous crack propagation. By evaluating the results, failure of the material can be investigated on a microscopic level.

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S04 | Structural mechanics

Organiser: Manfred Bischoff (*University of Stuttgart, Germany*)
Sven Klinkel (*RWTH Aachen University, Germany*)

S04.01 | Structural mechanics

Date: February 19, 2019
Room: Audimax

08:30-10:30

Transformations and enhancement approaches for the large deformation EAS-method

Robin Pfefferkorn (*Karlsruhe Institute of Technology, Germany*)
Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

08:30

The computer simulation of large deformation solid mechanics requires highly efficient finite elements. One widely used method enabling the construction of such elements is the enhanced assumed strain (EAS) method (cf. [3]). Although the EAS-method is well understood in geometrically linear-problems, there are still some issues in the geometrically nonlinear regime, which are addressed in this presentation. Different shape functions for the enhanced field are compared (see [4] and [2]), with focus put on the spurious hour-glassing problem. Furthermore, many transformations for the enhanced as well as the compatible deformation gradient have been used in previous publications (see e.g. [1]). We summarize these transformations and give new frame-invariant alternatives which fulfill the patch test and exhibit good bending performance. Finally, novel approaches for the enhancement are presented including enhancement of other kinematic measures than the deformation gradient. Numerical examples are presented to highlight the properties of various transformations, shape functions and enhancement approaches.

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On the relaxation of continuity conditions for finite element schemes based on a least-squares approach

Maximilian Igelbüscher (*University Duisburg-Essen, Germany*)
Jörg Schröder (*University Duisburg-Essen, Germany*)

08:50

The proposed contribution is based on the idea of the relaxation of continuity conditions and an enforcement of these continuity constraints for the considered fields via Lagrange multipliers. Therefore, a least-squares formulation depending on stresses and displacements $(\boldsymbol{\sigma}, \mathbf{u})$ is considered, which is defined by the squared $L^2(B)$ -norm applied to the first-order system of differential equation, here given by the balance of momentum and the constitutive equation,

compare for the case of linear elasticity e.g. [1]. In general the assumptions for the continuity conditions are related to the conforming discretization of the individual fields. For the underlying formulation the conforming discretization of displacements with polynomial functions of Lagrange type by \mathbf{u}_h in P_k demands continuity of the displacement field. Furthermore, a conforming approximation of the stresses, e.g. with vector-valued Raviart-Thomas functions, i.e. $\boldsymbol{\sigma}_h$ in RT_n , requires a normal continuity of the stresses. Here m denotes the polynomial order of the stress approximation and the interpolation order of the displacements are given by the index k .

A non-conforming discretization of the stresses considering discontinuous Raviart-Thomas approximation functions with $\boldsymbol{\sigma}_h$ in dRT_m yield to a relaxation of the continuity conditions. However an additional introduction of a Lagrange multiplier within the underlying least-squares formulation guarantee the fulfillment of the relaxed constraints. In addition to that a second approach with the non-conforming discretization of displacement and stress field as \mathbf{u}_h in dP_k and $\boldsymbol{\sigma}_h$ in dRT_m can be used. For the application of boundary tractions and the boundary displacements the same Lagrange multipliers are used. The idea of a non-conforming discretization and an application of Lagrange multiplier techniques for the ensurance of continuity are for example given for hybrid methods in [2, 3]. As a result of the discontinuous approximation of the stress as well as the displacement field a static condensation of the related fields can be performed for the global system of equations, which results in reduced system matrices. For the numerical analysis we consider as a foundation a two dimensional leastsquares element of type $RT_m P_k$.

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Selective strain scaling for tetrahedral finite elements

Anton Tkachuk (*University of Stuttgart, Germany*)

09:10

Manfred Bischoff (*University of Stuttgart, Germany*)

In many industrial simulations tetrahedral finite element meshes are unavoidable due to the complex geometry of bodies. Often, there is a need to combine these elements with explicit time integration schemes, like in simulation of wave propagation, crash-worthiness and metal forming. Therefore, there is a demand for accurate and efficient tetrahedral finite elements. In this contribution, a formulation with strain scaling to reduce locking for a tetrahedral finite element with Allman's degrees of freedom is proposed.

Performance of tetrahedral finite elements in the context of explicit dynamics is limited by locking or high CPU cost. One of the numerous possibilities to alleviate the problem of locking in finite elements is (selective) strain scaling. Compared to many other methods to avoid locking it has a couple of advantageous features. First, it does not introduce zero-energy modes. Second, it avoids additional degrees of freedom or solution of local equations, like for enhanced assumed strain formulations or the method of incompatible modes. Third, it is economical and can be used together with explicit time integration. In the current literature, two different approaches to selective strain scaling may be found. First, an algebraic approach, initially proposed for small-strain hexahedral finite elements by Sze, uses algebraic scaling of parasitic shear and normal strain components in natural coordinates. It was further developed for non-linear problems by Borrvall and implemented in LS-DYNA. It can be efficiently applied to hexahedral elements, where the parasitic strains are well studied and identified. Second, a variational approach uses

a general framework of variational templates as basis of high-performance finite elements by Felippa. Variational templates were applied to circumvent locking for co-rotational membrane and shell elements (Dal Cortivo et al.) and volumetric locking in solid elements by Felippa. These approaches are not limited to hexahedral elements and they are pursued here for a tetrahedral finite element with Allman's degrees of freedom. The influence of the technique on performance of the element in bending dominated load cases and on the critical time step illustrates the properties of the proposed element.

Application of the fast nonlinear analysis method on a clamped beam with a cubic spring

Özge Akar (*Friedrich-Alexander University Erlangen-Nuremberg, Germany*)

09:30

Kai Willner (*Friedrich-Alexander University Erlangen-Nuremberg, Germany*)

Numerical efficiency and thereby the reduction of calculation time for simulations are still considered very important despite the continuous improvement of computational capacities. This is why model reduction methods [1] have been used for decades and are still being developed further in many different areas of engineering. Civil engineering avails reduction methods for construction buildings in order to avoid unnecessary complexity in earthquake designing of structures. E. Wilson [3] carries out the determination of vibration modes by earthquake excitation by using Ritz vectors instead of the common Eigen vectors. Thus, only the modes of interest are obtained. Furthermore, he developed the Fast Nonlinear Analysis (FNA) method to easily insert nonlinearities like damping and base isolation in a construction model [3].

In the context of this work, the FNA method is applied on a finite element model of a clamped beam with a cubic spring that works at the free end of the beam. First, a harmonic excitement is applied and the vibration modes are obtained by using Ritz vectors. The calculation of Ritz vectors requires an iterative algorithm. A standard vector iteration algorithm is compared to the Krylov-based Arnoldi algorithm [2]. Thus, the model is reduced to a sufficient number of degrees of freedom. A piece-wise

exact integration method is implemented to iteratively determine the results for displacement, velocity and acceleration of the discretized beam. In order to prove the validity of the FNA method and to show the calculation time reduction, the results

are compared to those of a redundant model calculated with Newton Raphson method. Furthermore, measurements conducted on a real clamped beam model with a cubic spring provide experimental results that are compared to the computational results.

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Large deformation tangential-displacement normal-normal-stress elements

Astrid S. Pechstein (*Johannes Kepler University Linz, Austria*)

09:50

"Tangential-Displacement Normal-Normal-Stress" (TDNNS) elements have been introduced as mixed elements for small deformation linear elasticity. The major benefit of these elements is that they are free from shear locking in thin structures and volume locking for nearly incompressible materials.

In the current contribution, we extend these elements to the large deformation case. We use an updated Lagrangian setting to compute the displacement update from a consistent linearization of the nonlinear problem. The degrees of freedom are the tangential component of the displacement update in actual configuration, and the normal component of the Cauchy stress vector. We take special care to ensure that all terms arising in the principle of virtual works are well-defined in a mathematical sense, even though the displacement update is discontinuous.

As an application of high interest we propose to use these elements in electromechanically coupled simulations. It has been shown that they are highly suitable for the discretization of thin layered structures as are common in smart materials. We see that this benefit carries over to the large deformation case. When treating electro-active polymers, we observe good results also when the material becomes nearly incompressible.

The elements are freely available in the open source software package Netgen/NGSolve (see ngsolve.org).

Analysis-suitable CAD models based on watertight Boolean operations

Benjamin Marussig (*Technische Universität Graz, Austria*)

10:10

Benjamin Urick (*nVariate, USA*)

Elaine Cohen (*University of Utah, USA*)

Richard H. Crawford (*The University of Texas at Austin, USA*)

Thomas J.R. Hughes (*The University of Texas at Austin, USA*)

Richard F. Riesenfeld (*University of Utah, USA*)

Trimming procedures are ubiquitous in today’s engineering design, since they provide the basis for fundamental geometric operations such as Boolean operations. The resulting trimmed CAD models possess minor gaps and overlaps due to inevitable approximation errors and their current treatment in CAD systems. Hence, these models are not analysis-suitable in general. Trimming actually leads to several severe problems [1] and resolving them is one of the greatest challenges for the interaction of design and analysis.

An immense effort is necessary to make trimmed CAD models gap-free or “watertight” so that they can be used for simulations. In the context of conventional simulations, this is a mandatory part of the meshing process which leads to a complete reconstruction of the geometry. Alternatively, various isogeometric analysis concepts have been developed that aim to deal with the gaps during the simulation. In this work, we present another option that establishes a closer connection between design and analysis models, making a step towards an analysis driven design paradigm [2]. To be precise, geometric operations that yield analysis-suitable CAD models are proposed.

The corresponding watertight Boolean operations are built upon a novel strategy [3] that applies conventional user-defined tolerances of CAD systems in order to obtain conformal representations, thereby resolving the problems induced by trimming already during the construction of the design model. We discuss fundamental aspects of this construction of analysis-suitable CAD geometries and investigate their performance in isogeometric simulations. The proposed methodology is verified with a number of test examples considering potential and elasticity problems.

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S04.02 | Structural mechanics

Date: February 19, 2019

08:30-10:30

Room: SR 04

A meshfree method fulfilling the conditions on Galerkin solution schemes

Christian Weißenfels (*Leibniz Universität Hannover, Germany*)

08:30

Due to the accurate solution of differential equations in many cases and the simple imposition of boundary conditions the Finite Element Method is still the preferred solution scheme. However for many industrial applications, like jet cutting or additive manufacturing, due to the involved discontinuities such continuum based approaches are ill-suited. Meshfree methods are more advantageous since they simplify the modeling of fusion or cutting. In order to virtually reproduce the physics of such processes accurate meshfree methods are a prerequisite. Many different approaches were developed in recent years. However most of these violate one or more accuracy requirements and additional stabilization or correction schemes are necessary. An accurate solution cannot be guaranteed for any application with these approaches. Hence in this work a new solution scheme is developed. It is based on a Petrov Galerkin formulation of the Optimal Transportation Meshfree (OTM) method. The test function is discretized using a new formulation of local maximum entropy shape functions. This new solution scheme fulfills all conditions for Galerkin solution schemes and no additional stabilization or correction approach is necessary. Additionally boundary conditions can be imposed directly using this new solution scheme. It is shown that the new approach fulfills the patch test and leads to a converged behavior for the Cooks membrane and the punch test. Additionally, completeness conditions on test functions are formulated showing that the integration constraint, a necessary requirement on Galerkin solution schemes, corresponds to a special type of these conditions.

Peridynamic Petrov-Galerkin method: a generalization of the peridynamic theory of correspondence materials

Tobias Bode (*Leibniz Universität Hannover, Germany*)

08:50

Christian Weißenfels (*Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

The novel Peridynamic Petrov-Galerkin Method (PPG Method) is a stable and consistent, truly meshfree and not unphysically stabilized method, motivated by the concept of Peridynamics to formulate the balance of linear momentum in a non-local integral form. In the context of Peridynamics it is distinguished between two fundamental material modeling approaches: The first one is to derive the constitutive response from a non-locally distributed strain energy density function and the second one is, to use a locally defined strain energy density provided by the classical continuum mechanics. The PPG Method builds on the second approach with the assumption that the zero-energy modes in the peridynamic correspondence formulation are caused due to an inadmissible linearization. The generally non-linear deformation of the reference family H_0^k into the current configuration H_t^k is linear mapped by an averaged deformation gradient. This might be sufficient for local theories, but with increasing non-locality the produced error gets larger and results in zero-energy oscillations. Recent approaches of peridynamic higher order derivatives and subdivision-based Peridynamics do not suffer from zero-energy modes anymore have a more precise mapping (i.e. piecewise linear or quadratic). The PPG Method targets to accurately map the deformation of a family. A flexible and fundamental way to do this consists

of a Petrov-Galerkin method building on the local peridynamic linear momentum equation where different function spaces for the actual and virtual displacement are used to meet their specific requirements. On the other hand, this formulation allows it to consistently linearize the residual and to provide an analytical stiffness matrix which can also be used for the common peridynamic correspondence models where it is usually costly computed via Finite Differences.

Bulk and shear properties of architected, two-dimensional artificial materials as a function of their inner lattice design

Nikolaos Karathanasopoulos (*ETH Zurich, Switzerland*)

09:10

In the last decades, several inner unit-cell architectures have been studied as a basis for the design of artificial materials with tunable or enhanced mechanical properties. Amongst others, reentrant hexagonal, triangular, diamond, rectangular and chiral-shaped lattices have been studied. While a considerable emphasis has been posed on their effective normal loading properties, their shear and bulk attributes have received much less attention. The current work identifies two-dimensional lattice designs of low and high resistance to shear and bulk loads, computing and classifying the effective mechanical behavior of the previously mentioned lattice designs, with respect to the one observed for isotropic, common engineering materials, such as steel or concrete. The results indicate differences of orders of magnitude, depending on the artificial material's unit-cell design and on its lattice symmetry classification. Moreover, they suggest that the material's Poisson's ratio value is not a sufficient estimator of its shear attributes, unless an isotropic symmetry classification applies. What is more, it is shown that non-auxetic diamond-shaped lattice designs can be as shear-stiff or shear-stiffer than well-known auxetic lattice designs, such as reentrant hexagonal lattices, quantifying the relevant difference.

Energy absorption of re-entrant auxetic structures: a parametric study

Narasimha Rao Mekala (*RWTH Aachen University, Germany*)

09:30

Jannik Bühring (*RWTH Aachen University, Germany*)

Nima Jafarzadeh Aghdam (*RWTH Aachen University, Germany*)

Kai-Uwe Schröder (*RWTH Aachen University, Germany*)

In lightweight design different structural concepts are adopted to reduce weight and optimize the structural capacity concerning strength and stiffness. Recent years, one of the major adoption is developing and design of auxetic structures and materials. Auxetic materials/structures are a particular class of materials that have a negative Poisson's ratio. That means the material becomes thicker in the direction perpendicular to the applied force under tension. By virtue of this property, these structures and materials have generated considerable interest in the recent years because of their unique characteristics in contrast to the traditional engineering materials such as higher indentation resistance, higher fracture toughness and greater resistance to impact damage. Since the auxetic and non-auxetic materials exhibit different deformation mechanisms. Modeling of auxetic structures is of considerable importance and needs appropriate stress-strain configurations.

The present research is focusing on the better understanding of the behavior of the auxetic structures subjected to impact loads. Also, also the effect of several geometric parameters conferred with the material on its performance. Here, two different models, one with conventional and the other one is re-entrant auxetic structures resting on a rigid surface are studied under impact loading. Various results like the specific energy absorption, impact force, and force-displacement curves are predicted by performing numerical simulations in ABAQUS. Furthermore, some comparisons made with different parameters associated with the geometry to gain a better understanding of re-entrant auxetic structures under impact focusing on energy absorption characteristics.

Numerical investigations about the use of lattice structures in energy absorbing systems

Jannik Bühring (*RWTH Aachen University, Germany*)

09:50

Nima Jafarzadeh Aghdam (*RWTH Aachen University, Germany*)

Narasimha Rao Mekala (*RWTH Aachen University, Germany*)

Kai-Uwe Schröder (*RWTH Aachen University, Germany*)

The use of lattice structures in structural components is becoming increasingly important. Particularly in the field of topology and weight optimization in connection with additive manufacturing processes, such structures are indispensable in places where no solid material is needed.

For many components design freedom is often limited so that an improvement in structural properties must be achieved by choosing a different material or by adjusting material parameters. This is often associated with high costs and efforts, especially since materials are chosen not only on the basis of mechanical characteristics. With the use of lattice structures there are much more design parameters without the necessity of changing the outer structural dimensions.

Energy absorbing structures for crash or impact protection usually use deformation mechanism which are based on areal bending. In this work we show an alternative design concept for structural energy absorbing with the use of two and three dimensional cell arrays. Parametric studies show that there is a high influence of the design parameters on the total absorbed energy and on the time depending behaviour. It is shown that there is a high influence by activating alternative deformation mechanisms instead of or rather in addition to bending. This effect can be reached by the use of auxetic cell structures which have negative poisson ratios on a macroscopic view. With aimed adjustment of the cell parameters the effects of tension and bending can be influenced. To investigate the influences of the cell parameters on the absorption behaviour a parametric study is done for bending and stretching dominated cell arrays and the results are compared to each other.

Macroscopic modeling of open cell foams

Stephan Kirchhof (*TU Bergakademie Freiberg, Germany*)

10:10

Alfons Ams (*TU Bergakademie Freiberg, Germany*)

Open cell foams are widely used in engineering which includes an application in areas, where vibration excitations can act on the structures. Therefore dynamic properties as eigenfrequencies and natural modes are of great interest.

We will discuss the description of the dynamic behavior of open cell foams by stochastic macroscopic models. These are based on a computed tomography scan of the foam, which gives access to parameters and the power spectral density needed for the generation of the stochastic process. The simulation results shall be used to get an estimate of the natural frequencies and will be compared to the results of a vibration measurement on a real foam.

S04.03 | Structural mechanics

Date: February 19, 2019

16:30-18:30

Room: Audimax

A new approach to mixed methods for Reissner-Mindlin plates and shells

Walter Zulehner (*Johannes Kepler University Linz, Austria*)

16:30

A mixed method for Reissner-Mindlin plate/shell models is presented with the displacement, the bending moment, and the shear strain as unknowns. This mixed formulation is equivalent to the original primal formulation without additional regularity assumptions. For vanishing thickness the Kirchhoff-Love plate/shell model is recovered with the same function spaces for the displacement and the bending moment as for the Reissner-Mindlin model. The approach is related to some of the models presented in [1] and [2], where the displacement and a shear (or difference) vector are the unknowns. The resulting schemes proved to be free of transverse shear locking.

The practical implementation of the method is based on a Helmholtz-like decomposition of the bending moment, which allows the use of trial and test functions which are continuous but not necessarily continuously differentiable for discretization.

For the special case of plate models the approach leads to a partially decoupled system of second-order problems for which efficient solution strategies are available. This feature of the new approach was already observed in [3] for the Kirchhoff plate model.

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- [3] K. Rafetseder and W. Zulehner. A decomposition result for Kirchhoff plate bending problems and a new discretization approach. *SIAM Journal on Numerical Analysis*, 56(3):1961-1986, 2018.

Reissner-Mindlin shell theory based on tangential differential calculus

Daniel Schöllhammer (*Graz University of Technology, Austria*)

16:50

Thomas-Peter Fries (*Graz University of Technology, Austria*)

The classical approach of modelling shells is to introduce a local coordinate system resulting from a parametrization of the shell geometry [1]. This concept requires the introduction of co- and contra-variant base vectors and Christoffel symbols, which makes the approach less intuitive and more complex. Yet it has been the standard approach to simulate shells for the last decades. We propose a reformulation of the linear Reissner-Mindlin shell theory based on the tangential differential calculus (TDC). Then, all geometric quantities and resulting differential surface operators are based on a global Cartesian coordinate system. An advantage of this reformulation is that the requirement of a parametrized middle surface is circumvented which enables shell analyses on implicitly defined surfaces. Because the new formulation may be used no matter whether a parametrization is available or not, it may be seen as a generalization of the classical shell equations. Herein, the procedure presented in [2] for the Kirchhoff-Love shell is extended to the linear Reissner-Mindlin shell and the strong and weak form of the equilibrium are derived based on the TDC.

For the numerical simulation, the derived equations are discretized with the surface finite element method [3] using higher-order shape functions implied by Lagrange elements or NURBS patches.

In the case of parametrized surfaces, the approach is equivalent to the classical shell theory, however, the new formulation still implies a different implementation. Convergence analyses for numerous test cases are performed. The numerical results include classical and new test cases and higher-order convergence rates are achieved in the residual errors.

[1] M. Bischoff, K. Bletzinger, W. Wall and E. Ramm, Models and Finite Elements for Thin-Walled Structures, Encyclopedia of Computational Mechanics, John Wiley & Sons, Ltd, 2004 (Chapter 3).

[2] D. Schöllhammer, T.P. Fries, Kirchhoff-Love shell theory based on tangential differential calculus, Comput. Mech., submitted, 2018.

[3] G. Dziuk and C. Elliott, Finite element methods for surface PDEs. Acta Numerica, Vol. 22, pp. 289-396, 2013.

The Hellan-Herrmann-Johnson method for nonlinear shells

Michael Neunteufel (*TU Wien, Austria*)

17:10

Joachim Schöberl (*TU Wien, Austria*)

Finding appropriate discretizations for nonlinear shells is still a challenging problem. For Kirchhoff plates the Hellan-Herrmann-Johnson method introduces a moment tensor for computing the fourth order equation as a mixed method. The TDNNS method can be used to extend it to Reissner-Mindlin plates.

In this talk we present a generalization of these methods to nonlinear shells, where we allow large strains and rotations. We may assume the Kirchhoff-Love hypothesis to neglect shearing terms and focus on the bending energy, which is defined as the difference between the curvatures of the deformed and undeformed configuration of the shell. Therefore, we first show how the Weingarten tensor can be computed in a variational sense using $H(\text{divdiv})$ -conforming finite elements. Then we introduce the moment tensor as the Lagrange parameter of the curvatures. For the shearing term, we use $H(\text{curl})$ -conforming Nedelec elements for additional rotation degrees of freedom. With these elements, also non-smooth surfaces with kinks can be handled directly without rewriting terms.

The method is implemented in NGS-Py, which is based on the finite element library Netgen/NGSolve (www.ngsolve.org). Finally, we present numerical results.

A physically and geometrically nonlinear formulation for isogeometric analysis of solids in boundary representation

Margarita Chasapi (*RWTH Aachen University, Germany*)

17:30

Sven Klinkel (*RWTH Aachen University, Germany*)

This contribution concerns a physically and geometrically nonlinear formulation for isogeometric analysis of solids in boundary representation. The parametrization of the proposed approach is inspired by the scaled boundary finite element method, where the geometry of the boundary is sufficient to define the entire solid surface. This suits perfectly the boundary representation modeling technique, which is commonly employed for the design of solids in CAD. In order to provide a boundary-oriented approach, the solid surface is parametrized by a radial scaling parameter emanating from a scaling center and a parameter in the circumferential direction of the boundary. According to the idea of isogeometric analysis, NURBS basis functions define the geometry of the boundary and approximate the solution on the boundary. We also employ NURBS to approximate the solution in the scaling direction in the interior of the domain. This enables a straightforward treatment of nonlinear problems while preserving the exact geometry of the boundary. The approximation in scaling direction is in principal flexible and requires for coupling of adjacent patches inside the domain. The Galerkin method is employed for the

solution in both parametric directions and a linearization is derived which is used within an iterative Newton-Raphson scheme. We consider a wide range of nonlinear problems including elasto-plastic material behavior and large deformations as well as complex geometries commonly employed in engineering applications. Several benchmark tests are studied to evaluate the performance of the proposed approach.

[1] M. Chasapi and S. Klinkel. Isogeometric analysis of nonlinear elasticity - A Galerkin approach for boundary represented solids, submitted for publication.

[2] M. Chasapi and S. Klinkel. A scaled boundary isogeometric formulation for the elasto-plastic analysis of solids in boundary representation, *Comput. Methods Appl. Mech. Engrg.*, 333: 475-496, 2018.

[3] T.J.R. Hughes, J.A. Cottrell and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, *Comput. Methods Appl. Mech. Engrg.*, 194: 4135-4195, 2005.

Imperfection sensitivity of ring and stringer stiffened cylinders

Simon Kern (*Technische Universität Braunschweig, Germany*)

17:50

Dieter Dinkler (*Technische Universität Braunschweig, Germany*)

The buckling behaviour of thin shells which determines the load bearing capacity in many cases is profoundly influenced by perturbations of various types and requires computational analysis to take geometrical and physical non-linearities into account. When it comes to stiffened shells a significant increase in complexity of stability phenomena is observed. Therefore the formulation of general design recommendations is quite difficult and common standard specifications, which are still used in engineering practice, are based on experimental investigations. This may lead to very conservative and thus uneconomical design especially for stiffened shells. The sensitivity to imperfections can be evaluated using the perturbation energy concept which was introduced for a mixed finite element formulation. The concept allows to identify unfavourable non-initial perturbations which cause a snap through of the ideal structure on the basis of energetic considerations. No assumptions regarding the worst imperfection shape have to be made. A buckling criterion can then be formulated by comparing the calculated perturbation energy to experimental data. Since the perturbation load includes forces and strains it is not possible to use a common displacement based finite element formulation as the free variation of displacements and forces in the elastic potential is mandatory. Unfortunately mixed finite elements are disadvantageous for modelling stiffened shell structures since discontinuities of stresses can not be depicted without modifications. This problem is solved by application of the perturbation energy concept to mixed-hybrid elements. Because of the solely local definition of forces within the element domain the corresponding degrees of freedom can be condensed on element level and do not have to be continuous on the element border. Further advantages are the avoidance of shear and membrane locking and improved element behaviour for distorted meshes by the use of balanced shape functions. By adopting the semi-Loof concept for the rotational degrees of freedom the assembly of branched elements needs no special treatment even though only in-plane rotations are present. A validation of the mixed-hybrid approach is performed by solving the resulting non-linear quadratic eigen value problem for particular structures and comparing the results with solutions for mixed elements. The developed method is used to calculate critical perturbations for ring and stringer stiffened cylindrical shells and pointing out the crucial change of imperfection sensitivity due to the application of stiffeners. Depending on the analysed structure a positive as well as a negative influence can be shown.

S04.04 | Structural mechanics

Date: February 19, 2019

16:30-18:30

Room: SR 04

Modeling of NATM tunneling using a rock damage plasticity model

Magdalena Schreter (*University of Innsbruck, Austria*)

16:30

Matthias Neuner (*University of Innsbruck, Austria*)

Peter Gamnitzer (*University of Innsbruck, Austria*)

Günter Hofstetter (*University of Innsbruck, Austria*)

Predicting the complex mechanical behavior of a deep tunnel induced by NATM tunneling by means of finite element simulations requires appropriate constitutive models of the materials involved such as the surrounding rock mass or the tunnel support.

Rock is a frictional-cohesive material, characterized by a highly nonlinear stress-strain relation including hardening and softening material behavior. For realistic modeling of rock in simulations of deep tunneling, an isotropic rock damage-plasticity model was proposed in [1]. The model is formulated in the framework of continuum mechanics based on coupling plasticity theory and the theory of damage mechanics. In contrast to linear-elastic perfectly-plastic rock models, which are commonly used in practical applications, the rock damage-plasticity model predicts irreversible strains, strain hardening and strain softening material behavior including stiffness degradation. For regularizing the rock damage-plasticity model in the softening regime, a gradient-enhanced damage formulation was proposed in [2].

The rock damage-plasticity model was employed in 2D simulations of deep tunneling in [3]. Therein, during the excavation and securing process the formation of shear bands in the rock mass emanating from the tunnel surface was predicted, indicating potential failure of the tunnel. Nevertheless, in the 2D simulations several simplifying assumptions are made and complex construction sequences cannot be analyzed. Thus, in the present contribution the application of the rock damage-plasticity model to large-scale 3D finite element simulations of NATM tunneling is pursued, considering the real example of a stretch of the Brenner Base Tunnel. The numerical results of the 3D simulations are contrasted with those of the 2D simulations and are validated by comparison with displacement measurement data. Furthermore, the rock damage-plasticity model is evaluated by comparison with a commonly used linear-elastic perfectly-plastic rock model.

References

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[2] M. Schreter, M. Neuner and G. Hofstetter. “Evaluation of the Implicit Gradient-Enhanced Regularization of a Damage-Plasticity Rock Model”, *Applied Sciences* Vol. 8, No. 1004, 2018.

[3] M. Schreter, M. Neuner, D. Unteregger and G. Hofstetter. “On the importance of advanced constitutive models in finite element simulations of deep tunnel advance”, *Tunnelling and Underground Space Technology* Vol. 80, pp. 103-113, 2018.

Numerical modeling of shotcrete and application to simulations of deep tunnel advance

Matthias Neuner (*Universität Innsbruck, Austria*)

16:50

Magdalena Schreter (*Universität Innsbruck, Austria*)

Peter Gamnitzer (*Universität Innsbruck, Austria*)

Günter Hofstetter (*Universität Innsbruck, Austria*)

Shotcrete plays an essential role within the New Austrian Tunneling Method. Subsequent to each excavation step, a thin layer of shotcrete is directly applied onto the surrounding rock mass, forming a supporting shell which is usually loaded already several hours after casting due to further advance of the tunnel. Hence, the prediction of the mechanical behavior of this rock-support system is a time-dependent problem and demands for realistic constitutive modeling of shotcrete. The complex material behavior of shotcrete is characterized by the time-dependent evolution of material properties due to hydration, and by hardening and softening, creep and shrinkage.

Recently, in [1] a new constitutive model for shotcrete, based on a combination of the theory of plasticity, the theory of continuum damage mechanics, and a modified version of the solidification theory [2] was presented. The model represents the time-dependent material behavior of shotcrete, as well as hardening and softening material behavior.

In the present contribution, the application of the new model to a large scale simulation of deep tunnel advance together with an advanced material model for the surrounding rock mass is presented. To this end, a model derived from a stretch of the Brenner Base Tunnel considering the time-dependent construction process is developed. Based on the simulation results, the influence of the time-dependent, nonlinear material behavior of shotcrete on the structural response is discussed, and a comparison with available in-situ measurement data is presented.

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Multiphase simulations of concrete overlays interacting with an existing substrate

Andreas Brugger (*University of Innsbruck, Austria*)

17:10

Peter Gamnitzer (*University of Innsbruck, Austria*)

Günter Hofstetter (*University of Innsbruck, Austria*)

One of the most common measures for restoring and improving the load carrying capacity of reinforced concrete bridges is adding a concrete overlay. To allow an efficient design and dimensioning for this strengthening technique, it is necessary to appropriately consider the evolution of stiffness and strength as well as the shrinkage behavior of concrete overlays in interaction with an existing substrate. Thereby restraint effects in the form of tensile stresses in the overlay as well as compressive stresses in the existing bridge deck are induced, which are reduced over time by creep effects in compression and tension. Conventional models offer phenomenological descriptions of shrinkage and creep effects, but further basic research is required for a better understanding. Multiphase models promise an in-depth approach for numerical simulations of the placement of concrete overlays considering interactions with the substrate. Thereby the underlying coupled thermal, hygric, chemical and mechanical processes are described in detail based on the theory of partially saturated porous media. The early age properties are formulated in terms of the hydration degree. Shrinkage is described by means of the effective stress concept and creep on the basis of the microprestress-solidification theory. The governing equations represent balance of mass, momentum and enthalpy together with kinematic relations and constitutive laws for the individual phases.

The application of multiphase models for numerical simulations requires knowledge of a variety of parameters to realistically represent the respective mechanisms. Several comprehensive studies on a particular type of overlay concrete have been conducted, allowing calibration of a complete set of parameters and therefore an appropriate representation of the aforementioned coupled processes. In the present contribution a fully calibrated multiphase model is applied to

numerically investigate a brick-shaped specimen, which is supplemented by a concrete overlay. Thereby the water content distribution during the preparation of the top surface through wetting is examined, followed by an analysis of the temperature and moisture dependent hydration process after placement of the overlay. Subsequently the evolutions of shrinkage and creep strains in the composite specimen due to self-desiccation and drying are studied.

Concrete hinges: experiments, simulations, and design considerations

Thomas Schlappal (*TU Wien - Vienna University of Technology, Austria*) 17:30

Johannes Kalliauer (*TU Wien - Vienna University of Technology, Austria*)

Susanne Gmainer (*Smart Minerals GmbH, Austria, Camillo Sitte Lehranstalt, Austria*)

Markus Vill (*Vill Ziviltechniker GmbH, Austria*)

Josef Eberhardsteiner (*TU Wien - Vienna University of Technology, Austria*)

Herbert Mang (*TU Wien - Vienna University of Technology, Austria, Tongji University, China*)

Bernhard Pichler (*TU Wien - Vienna University of Technology, Austria*)

Concrete hinges are unreinforced or marginally reinforced necks in reinforced concrete structures. They were invented by Freyssinet in 1923. Practical applications include supports in integral bridge construction and segment-to-segment interfaces of segmental tunnel rings in mechanized tunneling. As for integral bridge construction, pioneering design guidelines were developed by Leonhardt and Reimann in 1965. They were adapted for the application in mechanized tunneling by Janßen in 1986, and translated into the nomenclature of modern European design standards by Marx and Schacht in 2010. Because this has raised the interest of structural engineers to gain more insight into the functionality of concrete hinges, both eccentric compression tests and cyclic bending tests under constant normal force were carried out in the research laboratories of TU Wien. Subjected to eccentric compression, the failure of concrete hinges is surprisingly ductile (Schlappal et al. 2017). In order to decipher the underlying mechanism, nonlinear three-dimensional Finite Element simulations were carried out by Kalliauer et al. (2018). The numerical analyses provided quantitative access to the triaxial stress states in the region of the neck, which are developing because the stress trajectories run around the notches of a concrete hinge. Still, biaxial compressive stress states prevail at the free lateral surface of the notch, at the compressed side of the concrete hinge. The biaxial compressive strength of concrete is reached quite soon in the structural bearing capacity test, but the layer of concrete at the surface does not spall away. This is why triaxial compressive stress states can be activated behind the surface layer, inside the volume of a concrete hinge. They explain the surprisingly high bearing capacity and the ductile behavior of concrete hinges. As for the application of concrete hinges in mechanized tunneling, the local behavior of segment-to-segment interfaces governs the overall structural behavior of segmental tunnel rings. This was quantified in the context of elastic limits and bearing capacities of segmental tunnel rings by Zhang et al. in 2018, who carried out structural simulations combining analytical solutions of the linear theory of slender circular arches with nonlinear interface models. In the present contribution, these developments are summarized and an outlook to the development of new design recommendations for serviceability limit states and ultimate limit states is provided.

S04.05 | Structural mechanics

Date: February 20, 2019

08:30-09:30

Room: Audimax

Combining of the machine learning algorithm with the optimal transportation meshfree (OTM) method for metal cutting simulation

Dengpeng Huang (*Leibniz Universität Hannover, Germany*)

08:30

Christian Weißenfels (*Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

The feed forward Artificial Neural Network (ANN) has been used as a tool for numerical modeling of non-linear material behaviors, such as elasto-plastic deformation. Unlike the classical plasticity model, the ANN-based material model does not require the local integration scheme and thus can speed up the metal cutting simulation. Additionally, if enough training data from experiments is obtained, the ANN model can be trained to express constitutive relationship accurately. In this case, the input data for the ANN is the strain components and the output data is the stress components. To capture the history dependent behavior, such as the plastic deformation with isotropic hardening, the stress and strain components in the last time step is usually included in the ANN inputs as well.

Instead of including only the last stress and strain as inputs of the feed-forward ANN, in this work, the Recurrent Neural Network (RNN) is applied to capture the history dependent elasto-plastic behavior, where the network has a longer memory of the history information. For training of this RNN based model, the inputs are the time series strain data in a sequence approach, where the history information are remembered by the network state calculated from the previous time steps. During the application, the total strain components are feed into the network according to the time sequence and the stress components can be calculated from the network outputs.

In this work, the ANN is trained by the data sets generated from the one-element boundary value problem with different loading paths. The ANN based material model is combined with the OTM method to simulate the metal cutting process.

Artificial neural networks in structural dynamics

Marcus Stoffel (*RWTH Aachen University, Germany*)

08:50

Franz Bamer (*RWTH Aachen University, Germany*)

Bernd Markert (*RWTH Aachen University, Germany*)

The aim of the present study is to identify a field of application for artificial neural networks in the prediction of complex structural deformations. Here, shock wave-loaded circular metal plates are considered, which deform viscoplastically during microseconds in an experimental set-up. A comparative study between finite element simulations and artificial neural network predictions is carried out. A geometrically non-linear first-order shear deformation shell theory in combination with a strain-rate dependent plasticity model and non-linear hardening is proposed for the finite element solutions. The numerical results based on artificial intelligence are obtained by a deep feed-forward neural network, developed in this study and trained by experimental data [1]. Moreover, by substituting the material law in the finite element code, a so-called intelligent element is developed [2], leading to finite element solutions combined with an artificial neural network. By comparing the numerical results to measurements in shock tube experiments, the accuracy of each approach is presented.

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Pseudo-kinematic invariants - gems in FE structural analyses

Herbert Mang (*Vienna University of Technology, Austria*)

09:10

Knowledge about invariants may considerably simplify their computation. The first invariants, students of mechanics are usually confronted with, are the three invariants of the stress tensor with respect to the coordinate systems used for their computation. Different from such invariances are the ones of the acceleration and the initial speed of a fictitious particle, moving non-uniformly on an originally unknown twisted curve on the unit sphere. These invariances are the hypothetical basis of an ongoing research project. They refer to an arbitrary real symmetric matrix as one of the two coefficient matrices of a class of linear eigenvalue problems in the framework of the Finite Element Method (FEM). The other one is the tangent stiffness matrix. The suspected invariant quantities are termed as pseudo kinematic because they are computed by a pseudo time that represents an arc length.

Contrary to the epistemological significance of the suspected invariances, their practical significance is, at first sight, rather limited. However, a mathematical expression, containing only the two invariant quantities, was recently shown by the author to be equal to the “non-membrane” percentage of the strain energy of shells, folded plates, arches, and frames. This theoretically remarkable and practically relevant result was obtained by solving the so-called consistently linearized eigenvalue problem, with the tangent stiffness matrix and its derivative with respect to a dimensionless load parameter as the two coefficient matrices. If the hypothetically assumed invariance of the aforementioned pseudo kinematic quantities can be verified, the second coefficient matrix, which generally must be approximated by a finite-difference expression, could be replaced by a simpler matrix –ideally by the unit matrix. The quoted mathematical expression would then remain valid, even if the tangent stiffness matrix was not differentiable, as may be the case for inelastic deformations.

To prove these invariances numerically, one special N-dimensional eigenvector each of two different linear eigenvalue problems will be used as a tool for determination of curves on the unit sphere, along which fictitious particles are moving. According to the underlying hypotheses, the acceleration and the initial speed of two corresponding 3-dimensional vectors, the vertices of which describe the two surface curves, should be equal.

The proof is part of ongoing research. If it is successful, topical program modules will be developed and subsequently implemented in a multi-purpose FE program system.

S04.06 | Structural mechanics

Date: February 20, 2019

14:00-16:00

Room: Audimax

Two novel Kirchhoff plate finite elements for the Modified Strain Gradient Theory

Murat Kandaz (*Middle East Technical University, Turkey*)

14:00

Husnu Dal (*Middle East Technical University, Turkey*)

Microplates are vastly used in MEMS and NEMS devices. Due to size effect, classical theories of continuum mechanics can not be used to model mechanical behaviour of them. Instead, higher order continuum theories should be implemented. Modified Strain Gradient Theory (MSGT) is considered to be one of the most accurate methods for this, considering both theoretical compatibility and numerical accuracy. In this study, two Kirchhoff bending plate finite elements for MSGT are developed as a novel aspect. This is done by first obtaining the weak forms by using variational methods and then deriving the set of algebraic equations for the finite element formulation, which are further solved by employing Gaussian quadrature. The length scale parameters for MSGT are identified for gold using the existing experimental results in literature. This study proposes the use of higher order theories for gold microplates for thicknesses small than 40 μm .

A rotation-free formulation of Mindlin's plate model

Manfred Bischoff (*University of Stuttgart, Germany*)

14:20

Bastian Oesterle (*University of Stuttgart, Germany*)

Plate and shell theories taking into account the effect of transverse shear deformation, sometimes denoted as Reissner-Mindlin models, have been around since more than half a century. For the special case of flat plates it is customary to use one displacement and two independent rotations as degrees of freedom in the corresponding mathematical formulation. One of the most important plate models of this type has been proposed by Mindlin and it will be taken as reference in the following.

In the literature, various attempts to formulate shear deformable plate models without using rotations can be found. Essentially, all of them rely on the idea of separating the deformation into a "bending displacement" and a "shear displacement", as it is almost trivially possible for shear deformable (Timoshenko) beams. None of them, however, exactly represents Mindlin's model.

The present study presents a rotation-free formulation that exactly reproduces Mindlin's plate theory. It reveals that a strict separation of the deformation into pure bending and pure shear parts is impossible in general. It is demonstrated that (and why) existing rotation-free shear deformable plate models therefore fail in certain situations. For example, they are not able to reproduce the typical boundary layer effects, present in Mindlin's plate theory.

Apart from the theoretical value of closing this gap in the literature, the rotation-free formulation has the benefit of being intrinsically free from transverse shear locking in the context of numerical solution schemes. This does not only apply to finite elements but it is independent of the discretization scheme, i.e. also meshless methods, collocation methods or any other discretization method show uniform convergence in the thickness, with no spurious stiffness and without the need to apply particular devices like reduced integration or mixed methods.

Rigorous amendment of Vlasov's theory for thin elastic plates on elastic Winkler foundations, based on the Principle of Virtual Power

Raphael Höller (*Vienna University of Technology, Austria*)

14:40

Mehdi Aminbaghai (*Vienna University of Technology, Austria*)

Lukas Eberhardsteiner (*Vienna University of Technology, Austria*)

Josef Eberhardsteiner (*Vienna University of Technology, Austria*)

Ronald Blab (*Vienna University of Technology, Austria*)

Bernhard Pichler (*Vienna University of Technology, Austria*)

Christian Hellmich (*Vienna University of Technology, Austria*)

Deflection modes relevant for plates with rigidly supported edges are commonly used as kind of “approximation” for the deformation behavior of plates which are freely swimming on an elastic foundation. However, this approach entails systematic errors at the boundaries. As a remedy to this problem, we here rigorously derive a theory for elastically supported thin plates with arbitrary boundary conditions, based on the Principle of Virtual Power. Somewhat surprisingly, it appears that the well-known Laplace-type differential equation for the deflections needs to be extended by additional boundary integrals entailing moments and shear forces, so as to actually “release” the boundaries from “spurious” acting external moments and shear forces. When approximating the deflections through 2D Fourier series, the Principle of Virtual Power yields an algebraic system of equations, the solution of which provides the Fourier coefficients of the aforementioned series representation. The latter converges, with increasing number of series members, to the true solution for the plate deflections. The new method is applied to relevant problems in pavement engineering, and it is validated through comparison of the numerical results it provides, with predictions obtained from Finite Element analysis. With respect to the latter, the new series-based method reduces the required computer time by a factor ranging from one and a half to almost forty.

An a-priori error estimate for the consistent approximation approach

Patrick Schneider (*Technische Universität Darmstadt, Germany*)

15:00

Reinhold Kienzler (*University of Bremen, Germany*)

The consistent approximation approach is a dimension reduction technique for the derivation of lower-dimensional analytical theories for thin structural members from the three-dimensional theory of elasticity. It has been successfully applied to a variety of problems by numerous authors. The approach is based on a structured truncation of the elastic energy. It has been shown that leading-order approximations for isotropic material deliver the known classical theories, like the Kirchhoff plate theory, or the Euler-Bernoulli beam theory, without invoking a-priori assumptions. On the other hand, the approach also allows to derive extended refined theories and/or theories for anisotropic materials in a systematic way. This has already been demonstrated by the authors for the case of a Reissner-type plate theory for monoclinic material.

In the talk, we show how the approach can be extended towards a simultaneous truncation of the dual energy, which allows for a structured derivation of compatible boundary conditions. Furthermore, using a duality principle, it is possible to provide an a-priori error estimate stating that the error of solutions of the arising hierarchy of approximating theories to the exact three-dimensional solution will decrease very fast with the order of approximation, if the structural member is sufficiently thin. Thus, the approximating character of the approach is proven. The procedure is demonstrated at the example of a one-dimensional, isotropic structural member with rectangular cross-section.

Linear elastic plates under in-plane action: unified analytical solution procedure based on displacement unknowns

Werner Guggenberger (*Graz University of Technology, Austria*)

15:20

In this paper in-plane plate problems under the geometrical-material conditions of small displacements and linear elasticity are considered. Furthermore, the existence of a uniform coordinate grid and grid conforming structural boundaries are presumed. Under such conditions, apart from some other restrictions, analytical solutions appear possible. These typical further restrictions appear procedurally necessary and relate to the type of uniformity of the coordinate grid and the prescription of boundary conditions in one of the two coordinate directions.

It has to be kept in mind that finally a system of partial differential equations (PDEs) will have to be solved, anyway. This appears rationally possible only if the problem is mathematically reduced to a final one - coordinate - dependency by introducing suitable product ansatz function systems. Then the system of PDEs becomes transformed into a system of ordinary differential equations (ODEs) which is basically open for applying analytical solution procedures.

Traditional structural engineering avoids any appearance of final 'systems' of differential equations. This led to the introduction of the (Airy) stress function approach in the present case which permitted dealing with one final system quantity only. Otherwise, this introduced many unwanted complications into the overall solution procedure for obtaining full information about section force quantities and displacement quantities.

In response to these undesired and disturbing inconsistencies, it is the dedicated aim of this paper to establish a unique procedure for problem formulation, as well as for analytical problem solution being uniformly based on deformation quantities, i.e. two displacement components in the present case. Thereby matrix representation is used throughout by intention. On the one hand, this permits obtaining a concise theoretical problem formulation, applying matrix differential operator notation. On the other hand, the steps of the analytical solution procedure for a single plate element, i.e. the formation of its element stiffness relationship and its related matrix quantities can be carried out in an elegant and consistent way.

Summing up, it turns out that the established procedure is problem - independent to a large extent. This holds not only in cases when the structural mechanical problem dealt with falls into the categories mentioned in the introduction, but even under much more general conditions which are designated by distinctly leading to a system of ODEs preferably with constant coefficients in the end.

The paper concludes with the demonstration of a few characteristic examples, e.g. the effective width problem or classical shear lag effect etc.

A closed-form analytical approach for stress concentrations at elliptical holes in moderately thick plates

Julian Felger (*TU Darmstadt, Germany*)

15:40

Wilfried Becker (*TU Darmstadt, Germany*)

Along with a progressively increasing use of lightweight design concepts, efficient and detailed methods for the analysis of stress concentrations, limiting the structure's load-bearing capacity, are desired. Based on classical works by Muskhelishvili [1] and Savin [2], the stress distribution around holes in plates under plane extension has been thoroughly investigated. However, an adequate treatment of open-hole plates under out-of plane or bending loading still raises difficulties. Classical Kirchhoff-Love plate theory lacks accuracy in the presence of sharp notches or holes with a characteristic length of the same order as the plate's thickness [3]. First-order shear

deformation plate theory (FSDT) yields adequate results but the governing system of partial differential equations impedes closed-form solution on complex domains.

The present work proposes a modified plate model situated in-between the established Kirchhoff-Love theory and FSDT. The modified plate model accounts for effects related to transverse shear deformation and allows the proper formulation of three physically sound boundary conditions. At the same time, the governing system of partial differential equations can be solved using a complex potential approach. Using the tool of conformal mapping, closed-form solutions are derived describing the distribution of bending moments and transverse shear forces at circular and elliptical holes. These findings are compared to results using classical Kirchhoff-Love plate theory as well as numerical data based on FSDT.

References

- [1] N. I. Muskhelishvili: Some basic problems of the mathematical theory of elasticity. Nauka, Moscow, 1966.
- [2] G. N. Savin: Stress distribution around holes. Naukova Dumka, Kiev, 1968.
- [3] S. P. Timoshenko and S. Woinowsky-Krieger: Theory of plates and shells. McGraw-Hill, 1959.

S04.07 | Structural mechanics

Date: February 20, 2019
Room: SR 04

14:00-16:00

Lattice Boltzmann simulation of the dynamic behavior of solids

Alexander Schlüter (*Technische Universität Kaiserslautern, Germany*) 14:00
Thomas Reinirkens (*Technische Universität Kaiserslautern, Germany*)
Charlotte Kuhn (*Technische Universität Kaiserslautern, Germany*)
Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

The Lattice Boltzmann Method (LBM) is mainly used to simulate fluid flows but can be applied to structural problems as well. In this work LBMs for solids under simplified deformation assumptions are investigated. In particular, the two-dimensional models of Guangwu [1] and Chopard et. al. [2] are analyzed. The standard formulations of these models are only able to describe mesh conforming geometries. However, it is possible to implement non-mesh conforming geometries within the LBM as well. This approach allows to model cracks in a more realistic manner, which is demonstrated by numerical simulations of several benchmark problems. Furthermore, the LBM results are compared to FEM simulation results in order to demonstrate the computational efficiency of the LBM.

- [1] Y. Guangwu, J. Comput. Phys. 161, 61-69 (2000)
- [2] B. Chopard, P. O. Luthi, Theo. Comput. Sci. 217, 115-130 (1999)

Inverse dynamics of underactuated flexible mechanical systems

Timo Ströhle (*Karlsruhe Institute of Technology, Germany*) 14:20
Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

Servo constraints have been successfully applied to solve the inverse dynamics of discrete mechanical systems. In this approach the equations governing the motion of the discrete mechanical system at hand are supplemented by algebraic servo constraints. The servo constraints serve the purpose of partially prescribing the motion of the mechanical system. The resulting set of differential algebraic equations (DAEs) has typically a differentiation index that ranges between three and five. After the application of index reduction techniques the DAEs can be solved by means of specific time-stepping schemes (see [1, 2] and references therein).

In principle the same approach can also be applied to the inverse dynamics of flexible mechanical systems such as elastic ropes and beams. To this end a discretization in space needs be applied first to generate the discrete mechanical system. Then servo constraints can be appended leading again to DAEs. However, the index of the resulting DAEs can be quite large hindering their numerical solution.

In our contribution we consider an alternative approach to the inverse dynamics of flexible mechanical systems. In contrast to a sequential discretization in space and time we apply a simultaneous space-time discretization of the problem at hand. In particular, we will compare a space-time finite element formulation with the method of characteristics. We will focus on mechanical systems whose motion is governed by quasilinear hyperbolic partial differential equations. Numerical examples are presented which underline the importance of solving this class of problems in space and time simultaneously.

[1] R. Seifried and W. Blajer. Analysis of servo-constraint problems for underactuated multibody systems. *Mechanical Sciences*, 4(1):113-129, 2013.

[2] R. Altmann, P. Betsch, and Y. Yang. Index reduction by minimal extension for the inverse dynamics simulation of cranes. *Multibody System Dynamics*, 36(3):295-321, 2016.

Comparison of different excitation strategies in Operational Modal Analysis (OMA)

Max Gille (*Technical University of Munich, Germany*)

14:40

Tobias Franz Christian Berninger (*Technical University of Munich, Germany*)

Daniel Jean Rixen (*Technical University of Munich, Germany*)

Different ways of exciting a structure for the use in Operational Modal Analysis (OMA) are compared and evaluated on a simple structure. As in OMA the exact excitation is unknown, some assumptions about the excitation have to be made and it is very hard or even impossible to meet all theoretical requirements, such as randomness of the excitation in time and space. As a result, compromises have to be made. Therefore, multiple techniques are evaluated to give a recommendation for those who want to perform OMA measurements themselves.

Classical Experimental Modal Analysis (EMA) is performed as a reference, and we compare these results with those of OMA with different types of excitation. These are: moving objects (e.g. finger, stick) tipping on the structure, scratching, brushing, and acoustic excitation with noise and different styles of music through a loudspeaker. In addition to the influence of the non-randomness, we will also investigate the effect of the measurement length on the accuracy of the identified modal parameters. In particular the variation of the identified modal damping will be considered, since it is often an important indicator for monitoring engineering systems. The experimental results are evaluated using LMS Test.Lab's (Operational) Modal Analysis toolboxes.

Design optimization of joint parameters using the frequency based substructuring approach

Ahmed El Mahmoudi (*TU Munich, Germany*)

15:00

Daniel Jean Rixen (*TU Munich, Germany*)

Dynamic Substructuring (DS) is a research field that has gained high attention in both science and industry. The aim of DS techniques is to provide engineers in structural vibrations and sound practical solutions to analyze the dynamic behavior of complex systems. This paper addresses the design optimization problem of joint parameters to reduce the magnitude of the total system response in the context of the Lagrange Multiplier Frequency Based Substructuring (LM-FBS)

coupling process. For illustration, we use rubber bushings from an automotive application in the field of noise, vibration and harshness (NVH). Depending on which parameters are changed on the respective rubber bushing, it has an influence on the sound pressure in the total vehicle system. By grouping the joints into engine mounts, front suspension and rear suspension mounts a method should be given to implement an optimization function within the LM-FBS approach. For this purpose, the rubber bushings are considered as a substructure using the pseudoinverse method, so that in order to determine the optimum parameters, an optimization function only has to be established for the substructure of the bushings in relation to the total system result.

The sudden release of a rod constrained by a sliding sleeve

Francesco Dal Corso (*University of Trento, Italy*)

15:20

Costanza Armanini (*University of Trento, Italy*)

Diego Misseroni (*University of Trento, Italy*)

Daive Bigoni (*University of Trento, Italy*)

A linearly elastic rod constrained by a sliding sleeve and with an attached mass at the free end is analyzed after its sudden release from the straight undeformed configuration when subject to a gravitational field. The equations of motion, derived from the principle of least action within a large rotation framework, show a jump in the internal axial action at the sliding sleeve exit as the result of the configurational force action. Towards the prediction of the structural system evolution, the governing equations are treated under the assumption of negligible rod's inertia. In particular, the numerical integration is performed in time solving a nonlinear differential-algebraic (DAE) system, considering the closed-form spatial integration in terms of the elastica. Two different possible evolutions for the system are distinguished for dimensionless loads above/below a transition value (dependent on the angle between the sliding sleeve direction and the gravity acceleration), as the final ejection/injection of the rod from/into the constraint. The theoretical predictions are corroborated by experimental tests performed on a realized physical prototype.

On nullity of homogeneous linearized kinematic and equilibrium equations of the system of supported and connected rigid bodies

Rado Flajs (*University of Ljubljana, Slovenia*)

15:40

The paper deals with the homogeneous linearized kinematic equations and the equilibrium equations of the system of supported and connected rigid bodies that occur at the undergraduate course of Statics in the first year of the study of Civil Engineering. In the paper the very fundamental relation $nullity(A) = nullity(B^T)$ is proven using the well known virtual work principle [1, 2]. Here, matrices A and B denote the matrix of the homogeneous linearized kinematic equations and the matrix of the equilibrium equations, respectively. However, despite the well known used techniques the proof is rather new and generally applicable, as opposed to the established approaches [3]. All theoretical proof steps are clearly illustrated with numerous selected working examples.

It is worth mentioning that the well known relation $A = B^T$ from [3] has not yet been confirmed. This equation is not even preferable for practical applications, because it imposes certain limitations on the number of equilibrium equations and unknowns. In the presented proof this relation is not needed. Simple relationship between matrices A and B was not found. However, the explicit relation between them can be constructed from the proof steps.

References:

- [1] G. Turk, M. Stanek, A method for determination of the regularity of the structure, Zeitschrift für angewandte Mathematik und Mechanik, ISSN 0044-2267, 1997, vol. 77, suppl. 1, p. 341-342
- [2] M. Stanek, G. Turk, A note on virtual displacements. V: Short communications in mathematics and mechanics, section 8-23, GAMM 99, Annual Meeting, University of Metz, France, April

12-16, 1999, (Zeitschrift für Angewandte Mathematik und Mechanik, ISSN 0946-8463, Vol. 80, suppl. 3). Berlin: Wiley-VCH, 2000, vol. 80, suppl. 3, p. 753-754

[3] A. Carpinteri, Structural mechanics: a unified approach, Oxford: Alden Press, London, 1997.

S04.08 | Structural mechanics

Date: February 20, 2019

16:30-18:30

Room: Audimax

Topology optimization combined with element-by-element solution techniques

Ramses Sala (*Technische Universität Kaiserslautern, Germany*)

16:30

Charlotte Kuhn (*Technische Universität Kaiserslautern, Germany*)

Christian Sator (*Technische Universität Kaiserslautern, Germany*)

Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

Topology optimization approaches are commonly used for design problems involving physical phenomena related to solid mechanics, acoustics, electromagnetism, fluid mechanics, and combinations thereof. In computational models of these physical phenomena the field variables are commonly approximated using spatial discretizations of the domain by means of the Finite Element Method. Even for topology design problems in which the field variables must only satisfy linear state equations, the solution of the resulting global system of equations can become a computational bottleneck. Because a high resolution spatial discretization of the design domain is often desired, the memory requirements for the global equation system can become huge, even when sparse matrix representations are used.

The aim of this work is to contribute towards improvements in efficiency and scalability of topology optimization approaches for large problems using parallel computing. This communication presents a topology optimization approach in which the Solid Isotropic Material with Penalization (SIMP) method [1] is combined, with Element-by-Element (EBE) solution techniques [2]. This approach reduces memory requirements since it does not require the assembly, storage, and solution of the the global system of equations. Because structured meshes are common in topology optimization also combinations of iterative EBE approaches with efficient solution techniques are investigated and compared against other modern and conventional topology optimization approaches.

References:

[1] Bendsøe, M. P. (1989). Optimal shape design as a material distribution problem. Structural optimization, 1(4), 193-202.

[2] Hughes, T. J., Levit, I., & Winget, J. (1983). An element-by-element solution algorithm for problems of structural and solid mechanics. Computer Methods in Applied Mechanics and Engineering, 36(2), 241-254.

Topology optimization with geometrical nonlinearity responding to uncertain loading

Junji Kato (*Nagoya University, Japan*)

16:50

Takayuki Nishino (*Tohoku University, Japan*)

The present study proposes a topology optimization method considering finite deformation for uncertain loading conditions. The loading angle is assumed to be uncertain as a condition. The objective is to minimize expectation and standard deviation of end-compliance obtained by means of a Total Lagrangian finite element formulation. In this case, it is not easy to derive an

analytical estimation of the expectation and the standard deviation because of its mathematical complexity. In order to solve this problem, we approximate the end-compliance by a Taylor series expansion and derive the mathematical formulation. In this approach, the second derivative of the objective function is necessary to hold the accuracy in sensitivity. The cause of errors which increase as the deviation gets larger and the scope of the application of this method are investigated in terms of numerical validations. Finally, some numerical examples demonstrate the usefulness of the proposed method.

Redundancy distribution in structures

Malte von Scheven (*University of Stuttgart, Germany*)

17:10

Florian Geiger (*University of Stuttgart, Germany*)

Jan Gade (*University of Stuttgart, Germany*)

Ekkehard Ramm (*University of Stuttgart, Germany*)

Manfred Bischoff (*University of Stuttgart, Germany*)

For the design of load bearing structures redundancy and thus the degree of static indeterminacy plays an important role. According to Linkwitz and Ströbel the distribution of static indeterminacy in the system can be described by the redundancy matrix containing the redundancy contributions of all element. The redundancy contribution of one element quantifies the internal constraint of the surrounding structure on this element. The sum of the redundancy contributions of all elements is equal to the degree of indeterminacy of the entire structure. The extension of this notion presented by Ströbel for discrete truss systems to frames and continua can yield valuable insight into the load bearing properties of a structure and has the potential to become an exciting new branch of the classical field of structural analysis.

The redundancy calculation for truss and frame structures will be explained and mathematical and mechanical properties of the redundancy matrix will be discussed.

A variational formulation for motion design of adaptive structures

Renate Sachse (*University of Stuttgart, Germany*)

17:30

Manfred Bischoff (*University of Stuttgart, Germany*)

In contemporary architectural structures, energy efficiency and sustainability plays an important and further growing role. This is why architects and engineers are determined to design extremely efficient structures. One possibility to meet this condition is to make use of adaptivity.

One type of adaptive structures is designed to adjust to varying loading. Optimal geometries for the different dominating load cases can be provided by classical structural optimization. The transition between those geometrical configurations is mostly characterized by small displacements where linear analyses are sufficient.

Another purpose of adaptive structures is the adjustment to changing requirements that occur during usage of the building. Examples for this are deployable and retractable structures, for opening and closing of façades or roofs, where the geometries of the different configurations differ significantly from each other. Here, not only the geometry itself needs to fulfil specified requirements, but also the shape transition has to be designed to satisfy the condition of efficiency. These motions include large displacements and therefore geometrically nonlinear analyses need to be considered. This contribution deals with such shape transitions as a motion between two (or more) geometrical configurations and their design, based on a variational formulation.

As an illustration example, we first refer to the Brachistochrone curve, which represents one of the first problems solved by variational principles. For the motion design the functional is defined as the particular quantity related to the motion that needs to be minimized. The method is developed with the exemplary condition of minimization of the strain energy during the whole

deformation process. By a discretization of the motion path with finite elements, additionally to the spatial discretization, a linear system of equations is obtained.

The proposed method is verified by means of applications with known exact solutions, for instance the motion of a kinematic system with zero strain energy throughout the entire process. With this method, various movements with different properties can be designed.

Phase field modeling with IGA and FEM: Error surveillance in the transition zone

Markus Klassen (*RWTH Aachen University, Germany*)

17:50

Ingo Münch (*Karlsruhe Institute of Technology, Germany*)

Sven Klinkel (*RWTH Aachen University, Germany*)

In the context of numerical methods, phase field models allow to capture the transition of phases which can occur in solid structures. To this end, a phase field variable is introduced in the mechanical model which is then coupled to the main solution field like e.g. the displacement. Furthermore, the evolution of the phase field is computed by a proper time integration scheme. This allows to simulate phenomena such as solid-state phase-transformations, solidification processes, crack propagation and others.

The present contribution compares the solution of a phase field problem by the finite element method (FEM) with isogeometric analysis (IGA). For the sake of simplicity, the coupling to additional fields is neglected. Thus, the phase field variable appears as the only unknown in the boundary value problem. The numerical solutions are compared to the analytical solution, elaborated by Falk, of the Allen-Cahn equation. In this model, the Ginzburg-Landau free energy density combines a free Landau energy of sixth order with a quadratic gradient energy. The benchmark consists of a simple quadrilateral geometry with boundary conditions for the phase field variable which allows to solve static unidirectional phase transitions. For the FEM, the mesh is refined uniformly in space by h- and p-refinement. In IGA, the refinement is realized by the knot insertion and order elevation algorithms from computer aided design (CAD) which is known as k-refinement. Furthermore, IGA allows for a higher continuity between the elements which enhances the gradient of the phase transition variable.

The talk will introduce the fundamental concepts of IGA and phase field modeling. Afterwards, the numerical implementation and simple benchmarks will be presented in order to show the capabilities of the method. Finally, the presentation will be closed by concluding remarks and future perspectives.

Topology optimization with isogeometric analysis and phase field modeling

Ingo Münch (*KIT, Germany*)

18:10

Markus Klassen (*RWTH Aachen, Germany*)

Werner Wagner (*KIT, Germany*)

We present a Phase Field Model using Isogeometric Analysis for the evolution of load-bearing solid structures with linear elastic material. The model generates structures with help of a sensitivity function accounting for equivalent stress. Similar to Evolutionary Structural Optimization (ESO) a threshold of equivalent stress is evaluated using information from all integration points. The user of the model has to consider the desired material proportion within the design space, which is a side condition to the optimization process. The evolution of material is ruled by an Allen-Cahn equation and the state of equivalent stress. The variational approach drops conservation of mass, and couples density as well as stiffness of the continuum by the phase field variable. Material and voids separate from an initial state of homogeneously distributed material. Thus, the model is able to deal with topological changes and yields the nucleation of holes.

In our numerical examples we compare the solution of the phase field model solved by the Finite Element Method (FEM) and with Isogeometric Analysis (IGA). Latter allows for a higher continuity between the elements which enhances the gradient of the phase transition variable. This is helpful to avoid the well-known mesh-pinning effect in phase field modeling.

Additionally, we modify the Laplacian operator in the phase field equation as proposed by Takaki and Kato [1]. The curvature of the phase transition zone between material and void usually yields a contribution to the free-energy of the system. This results in rounded shapes at the intersection of beam-like topologies, which is unrequested in certain cases. Another numerical example discusses that issue.

[1] T. Takaki and J. Kato: Phase-field topology optimization model that removes the curvature effects. *Mechanical Engineering Journal* 4(2), 16-00462, 2017.

S04.09 | Structural mechanics

Date: February 20, 2019

16:30-18:30

Room: SR 04

Prediction of stress states in tramway rails by means of a principle of virtual power-based, enhanced beam theory approach

Patricia Hasslinger (*TU Wien - Vienna University of Technology, Vienna, Austria*) 16:30

Christian Hellmich (*TU Wien - Vienna University of Technology, Vienna, Austria*)

Stefan Scheiner (*TU Wien - Vienna University of Technology, Vienna, Austria*)

In urban areas, tramways are an important means of transportation, demanding high reliability and safety of the tramway network. Tramway rails are typically embedded in the road, and exhibit a distinctive groove guiding the tramway wheels, implying asymmetric shapes. Failures of such rails are clearly caused by excessive mechanical loading due to tramway operation, but are decisively influenced by a range of additional factors. The latter include eigenstresses which are induced in the course of the manufacturing process and which may (significantly) change over the service life of the rails. Furthermore, stresses due to temperature changes may play an important role. As regards the rail itself, the condition of the track bed, as well as rail wear effects may strongly influence the resulting stresses in the rails. Surprisingly, studies elucidating the stress states which lead to cracks or even fractures in tramway rails, taking the aforementioned aspects into account, have been neglected so far.

This contribution focuses on the determination of the mechanical stresses in tramway rails, considering boundary and loading conditions which are representative for tramway operation. For that purpose, an enhanced beam model considering axial, shear, bending, primary and secondary torsional deformation were derived in the framework of the principle of virtual power (PVP). Considering beam kinematics inspired, on the one hand, by the well-known pioneers of beam theory, namely by Euler, Bernoulli, and Saint Venant, and, on the other hand, also by the more recent works of Sapountzakis (*ISRN Civil Eng, Article ID 9165, 2013*) and Gruttmann (*Int J Numer Method Eng, 45: 865-889, 1999*), in the fundamental equations of the PVP gives access to the governing equilibrium conditions and stress resultants of the tramway rail-representing beam. The resulting equations were solved by means of the Finite Element (FE) method, using linear and cubic shape functions for the interpolation between the nodal values of the beam-specific degrees of freedom, including the translational and rotational deformations with respect to all spatial directions, as well as the twist. The such obtained internal forces allow for calculating the cross-sectional distributions of normal and shear stresses along the beam axis - the cross-sectional boundary value problems were solved by means of 2D FE approximations.

Evaluating the model, critical boundary and loading conditions can be identified, potentially leading to rail failures. Compared to full 3D FE simulations, our approach offers the advantages of higher model flexibility, and, importantly, of substantially increased computational efficiency.

Role of diameter and percentage of SMA bars as reinforcement in strength and residual displacement of concrete beams

Mohammad Amin Esmail Molod (*TU Dortmund, Germany*)

16:50

Franz-Joseph Barthold (*TU Dortmund, Germany*)

Panagiotis Spyridis (*TU Dortmund, Germany*)

Concrete reinforced with conventional steel bars has been the most common construction materials for decades. Although it has some weaknesses that lead to some structural failures every year, it is still used to construct a wide range of bridges, buildings and routes around the world. One of those weaknesses is appearing cracks at the early age of service life of the structures. This phenomenon is inevitable, but some ideas have been proposed by scholars to mitigate its damage's intensity and consequences. One of those ideas is to use intelligent materials with specific features like self-sensing, self-repairing and actuating within concrete members; this technique leads to have smart structures. One of those smart materials that has currently attracted special attention of researchers in field of civil and structural engineering is shape memory alloy (SMA). There are two different forms of SMA; 1) superelastic shape memory alloy and 2) shape memory effect. Superelastic SMA made of Nickel-Titanium known as Nitinol is the most common and applicable kind of SMA in civil engineering. This kind of alloy can be embedded into concrete beams as reinforcement to help the beams recovering their initial form after undergoing to large deformations. Many experimental studies in this regard have been done, but only few numerical investigations. In addition, there is still doubt in choosing suitable ratio, shape and thickness of the SMA bars as reinforcement of the concrete beams. Hence, the author will concentrate on a numerical study in order to find out influence of percentage and thickness of the SMA bars on stiffness, residual displacement, recovery ratio and cracking load of the beams.

To do so, eight beams with same geometry $500 \times 100 \times 100$ mm and simply supported boundary condition under four-point bending test have been simulated via Ansys APDL software. Two load cycles with duration of 60s for each cycle, 30s loading and 30s unloading, were applied on top surface and $L/3$ distance from side of the beams. Two cases of study are taken into consideration; six beams reinforced with different percentages of SMA, but same diameter as first case and three beams with different diameters, but same percentage as second case. Results have shown that enhancement of ratio of SMA in the beams will reduce residual displacement and increase stiffness, cracking load and recovery ratio of the beams, while thickness of the bars will not affect the results significantly.

Effect of uncertain parameters on the deflection of beams

Thomas Reppel (*Universität Siegen, Germany*)

17:10

Tim Fabian Korzeniowski (*Universität Siegen, Germany*)

Kerstin Weinberg (*Universität Siegen, Germany*)

In classical beam theory, the deflection w depends on different parameters. On the one hand we have material and geometric parameters, like the Young's Modulus E , the second moment of area I and the length of the beam l . On the other hand there are different loading types like point loads F , distributed loads, or varying loads. All these parameters are usually modeled in a deterministic way.

In this contribution we analyze the distribution of the beam deflection w at certain points depending on uncertain, noisy parameters. To this end we model the parameters as random variables

(F, l) or random fields (EI) of different distributions. For this uncertainty we identify the resulting distribution types of the deflection. In the case of random fields, we also perform a parameter study to investigate the influence of the refinement to the resulting distributions.

Non-material finite element rod model for out-of-plane bending of an elastic strip with natural curvature

Christian Schmidrathner (*TU Wien, Austria*)

17:30

Yury Vetyukov (*TU Wien, Austria*)

A novel finite element formulation for elastic unsharable rods in the three-dimensional space is presented. Looking forward to future implementations of axially moving belts, we use a mixed Eulerian-Lagrangian kinematic formulation, which has the advantage that the element nodes are fixed in one spatial coordinate and the material points are flowing through it, hence it is possible to discretize the free elements coarser than the ones in contact with the pulleys. In this talk we present the solution of hanging rods with a flat cross-section including a natural curvature, which causes an out-of-plane bending as well as torsion of the rod. For validation purposes we limit ourselves to equilibrium solutions (at which purely Lagrangian elements would be also good enough) with clamping boundary conditions. The results are compared with both, the shell model of the hanging strip and the semi-analytical solution of the boundary value problem of the rod considering the natural curvature as small. Preliminary results concerning the contact problem for a steel belt hanging on two pulleys are discussed.

Comparison of performance and accuracy of the FETI-methods and a direct sparse FE-solver for truss structures

Corinna Barbara Schmaußer (*Technical University of Munich, Germany*)

17:50

Gerhard Müller (*Technical University of Munich, Germany*)

In the presented paper, the four Finite Element Tearing and Interconnecting (FETI) methods “Standard FETI” (FETI-1), “Two-Level FETI” (FETI-2), “Dual-Primal FETI” (FETI-DP) and “Total FETI” (TFETI) are applied for truss structures. The FETI methods are non-overlapping domain decomposition methods with Lagrange multipliers introduced at the substructure interfaces to enforce the continuity of the displacement field. They are in general highly efficient due to their suitability for the fast sequential and parallel iterative solution of large-scale second-order and fourth-order elasticity problems. In the study, the applicability, robustness, efficiency and accuracy of the FETI methods for truss structures of various sizes (large-scale and small-scale problems) under static loads in dependence of the chosen substructuring is investigated and compared with a standard FE-solver.

Shape memory alloy truss lattice material

Mieczyslaw Kuczma (*Poznan University of Technology, Poland*)

18:10

We will present a mathematical model and its predictions for the shape memory alloy truss lattice material in the range of pseudoelasticity. The proposed model is based on the ideas and concepts presented in Ref. [1,2,3] and extends them into the range of pseudoelastic (superelastic) behaviour [4,5]. Use is made of the Clausius-Duhem inequality in order to control the dissipation of energy during the deformation process, which allows us to consistently formulate the progress of martensitic phase transformation process in the members of the truss lattice material as a complementarity problem, and to effectively describe the characteristic flag-type hysteresis loops in the stress-strain space. Both small-strain and large-strain kinematics were considered.

The author developed a FE computer programme for this type of material structure. The obtained numerical results show that a pseudoelastic shape memory alloy truss lattice material will exhibit a sequence of hysteresis loops, when subjected to a closed-cycle loading programme, which demonstrate the large damping capacity of the material.

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S04.10 | Structural mechanics

Date: February 21, 2019
Room: Audimax

08:30-10:30

Structure-preserving integrators for discrete mechanical systems subject to general holonomic constraints

Alexander Janz (*Karlsruhe Institute of Technology, Germany*)

08:30

Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

Energy-momentum consistent (EMC) schemes constitute a specific class of structure-preserving integrators which have been primarily developed in the framework of non-linear structural dynamics.

EMC schemes are known for their superior numerical properties in terms of stability and robustness, see Betsch (Structure-preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics. Volume 565 of CISM Courses and Lectures. Springer-Verlag, 2016) for more details concerning these integrators.

EMC schemes typically rely on the notion of a discrete derivative which is applied to the stored energy function of the underlying continuum theory (e.g. nonlinear elastodynamics, geometrically exact beams and shells). In the presence of holonomic constraints the discrete derivative is also applied to the corresponding constraint functions to yield EMC schemes for constrained mechanical systems (such as multibody systems).

In its original form the discrete derivative concept is confined to functions that can be written in terms of invariants that are at most quadratic in the state variables, see Gonzalez (*J. Nonlinear Sci.*, 6: 449-467, 1996). The invariants are related to specific symmetries of the underlying mechanical system implying the conservation of associated momentum maps.

However, there exist specific problems in non-linear dynamics (e.g. contact problems), in which the relevant invariants are cubic functions of the state variables. We present an extension of the previous approach to the design of EMC schemes to cope with the general problem of discrete mechanical systems with symmetry. Our new developments are illustrated within the model problem of a Cosserat point.

GENERIC consistent discretisation in space and Energy-Momentum-Entropy consistent schemes for open thermomechanical systems

Mark Schiebl (*Karlsruhe Institute of Technology, Germany*)

08:50

Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

This work deals with the Energy-Momentum-Entropy (EME) consistent discretisation of open thermoelastic systems in space and time. While Energy-Momentum (EM) consistent numerical methods are well-known for conservative mechanical systems, Romero introduced in (Ignacio Romero. Thermodynamically consistent time-stepping algorithms for non-linear thermomechanical systems. *International journal for numerical methods in engineering*, 79(6):706-732, 2009) the class of thermodynamically consistent (TC) methods for coupled thermomechanical systems, which comply with the first and second law of thermodynamics. If a TC method respects the symmetries of the underlying system as well it can be viewed as an extension of EM methods to the dissipative regime and thus could be termed Energy-Momentum-Entropy consistent method. The construction of EME methods is based on thermodynamically admissible evolution equations expressed in the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) framework, originally proposed by Grmela and Öttinger (Miroslav Grmela and Hans Christian Öttinger. Dynamics and thermodynamics of complex fluids. i. development of a general formalism. *Physical Review E*, 56(6):6620, 1997). This double generator formalism relies on the additive decomposition of the evolution equations into reversible and irreversible contributions and is independent of the specific choice for the thermodynamical state variable (see Alexander Mielke. Formulation of thermoelastic dissipative material behavior using generic. *Continuum Mechanics and Thermodynamics*, 23(3):233-256, 2011).

We explore the structure of the GENERIC framework using the entropy density (see e.g. M Krüger, M Groß, and P Betsch. An energy-entropy-consistent time stepping scheme for nonlinear thermo-viscoelastic continua. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, 96(2):141- 178, 2016), the absolute temperature (see e.g. Markus Hütter and Bob Svendsen. Thermodynamic model formulation for viscoplastic solids as general equations for nonequilibrium reversible-irreversible coupling. *Continuum Mechanics and Thermodynamics*, 24(3):211-227, 2012) and the internal energy density, first for finite-dimensional systems in matrix-vector representation and then for infinite-dimensional systems in bracket form.

The infinite-dimensional systems is discretised in space leading to a finite-dimensional systems which can be expressed in the matrix-vector representation of the GENERIC where a GENERIC consistent spatial discretisation is introduced. Applying the notion of a discrete gradient (Oscar Gonzalez. Design and analysis of conserving integrators for nonlinear Hamiltonian systems with symmetry. PhD thesis, Stanford University Stanford, CA, 1996) leads to EME consistent methods.

The presentation will also address the impact of the choice of thermodynamical variable on the numerical method. In particular, either the total temperature, the entropy density or the internal energy density are used as thermodynamical state variable.

An alternative conservative/dissipative time integration scheme for nonlinear mechanical systems

Cristian Guillermo Gebhardt (*Leibniz University of Hannover, Germany*)

09:10

Raimund Rolfes (*Leibniz University of Hannover, Germany*)

A key aspect to produce acceptable numerical results in the context of conservative mechanical systems is the exact preservation of first integrals of motion like the total energy and/or even the

preservation of the underlying symplectic form that does exist in the continuous setting. The conservation of linear and angular momenta as well as relative equilibria is only warranted when the formulation adopted is based on objective deformation measures that are invariant under rigid body motion. In the numerical context, the conservation properties ensure that beyond the approximation errors due to the discretization, the computed solution remains consistent with respect to the underlying physical structure. The construction of numerical schemes showing the preservation of one or several of these properties is not an easy task. It comprises finding discrete versions of the continuous terms. After evaluating them at the time-quadrature points and in combination with appropriate admissible discrete variations of the generalized coordinates and the generalized velocities, they ought to guarantee “by design” the desired conservation features. For nonlinear systems, this is not directly achieved just by evaluating the continuous terms at the temporal collocation points, because the consistency and directionality conditions of the discrete derivatives are not automatically satisfied. Therefore, the involved discrete setting ought to parallel the continuous framework. Moreover, it is well-known that not all mechanical invariants can be discretely preserved for a fixed time step. The concomitant preservation of the total energy and the symplectic form is only achieved by adaptation of the time step, whose size is obtained by solving an optimization problem subjected to inequality time constraints, or by a discrete redefinition of the potential function.

Here, we present an alternative conservative/dissipative temporal integration scheme for nonlinear mechanical systems, which provides algorithmic forces and velocities that warrant desired conservation/dissipation properties. Our approach relies on a collection of linearly constrained quadratic programs especially formulated to minimize discrete perturbations. Such perturbations are aimed to correct deficiencies of the discrete terms. The solution of these programs provides explicit formulas for the algorithmic forces and velocities, which can be easily incorporated into existing implementations. Similarities and differences of our approach with respect to well-established methods are discussed as well. Finally, the approach, which is suitable for reduced-order models as well as for finite element models or multibody systems, is tested with examples of increasing difficulty.

Mixed frameworks and structure preserving integration for coupled electro-elastodynamics

Marlon Franke (*Karlsruhe Institute of Technology, Germany*)

09:30

Rogelio Ortigosa (*Polytechnic University of Cartagena, Spain*)

Alexander Janz (*Karlsruhe Institute of Technology, Germany*)

Antonio J. Gil (*Swansea University, United Kingdom*)

Peter Betsch (*Karlsruhe Institute of Technology, Germany*)

In the present contribution new approaches for the design of structure preserving time integrators for nonlinear coupled problems are proposed. Polyconvexity inspired energy functionals are obtained by using the rediscovered tensor cross product which greatly simplifies the algebra, see [1]. In this connection an extended kinematic set, consisting of the right Cauchy-Green tensor, its co-factor and its Jacobian, is introduced. On this basis coupled problems like e.g. non-linear thermo-elastodynamics, see [2] or electro-elastodynamics, see [3], can be considered. Furthermore the formulations are readily extendible for mixed Hu-Washizu type formulations where the extended kinematic set is introduced as unknown field. In particular in [1] an elegant cascade system of kinematic constraints was introduced for elastodynamics, crucial for the satisfaction of the required conservation properties of a new family of energy momentum (EM) consistent time integrators. The objective of the present contribution is the introduction of new mixed variational principles for EM consistent time integrators in electro-elastodynamics, hence bridging the gap between the previous works [3] and [1], opening the possibility to a variety of new finite element implementations, see [4]. The following characteristics of the proposed EM consistent

time integrator make it very appealing: (i) the new family of time integrators can be shown to be thermodynamically consistent and second order accurate; (ii) piecewise discontinuous interpolation of the mixed fields is carried out in order to obtain a computational cost comparable to that of standard displacement, electric potential formulations. Eventually, the superior performance of the proposed formulations is shown in several numerical examples.

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- [3] Ortigosa, R., Franke, M., Janz, A., Gil, A. and Betsch, P., An energy-momentum integration scheme based on a convex multi-variable framework for non-linear electro-elastodynamics, *Comput. Methods Appl. Mech. Engrg.*, 339:1-35, 2018.
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A numerical approach for dynamic analysis of solids in boundary representation

Arturo Mendez Salas (*RWTH Aachen University, Germany*)

09:50

Margarita Chasapi (*RWTH Aachen University, Germany*)

Sven Klinkel (*RWTH Aachen University, Germany*)

This contribution is concerned with a numerical approach for the dynamic analysis of solids in boundary representation. The proposed approach is based on the principle to represent a computational domain by scaling its boundary with respect to a scaling center, see [1] and the references therein. In CAD solids are defined through their bounded surfaces. Hence, the present method is perfectly suited to analyze such structures. The present work is restricted to the 2D case. For the adopted representation, the NURBS are used as basis functions to depict the complete domain geometry, as well as to approximate the unknown field variables of the problem. The adopted approach aims to provide accurate results for the dynamic analysis in cases where only the boundary of the geometry is available. Moreover, the aim of this approach is also supported by taking into account the advantage of the high continuity and nature of the used interpolation functions. For this formulation, the weak form of the equilibrium is enforced in the entire domain, which is represented by an elastic, homogeneous and isotropic medium. The Gauss integration method is used to solve the weak form of equilibrium. As an extension, a damped system is also considered for certain examples. Hence, the approximation of the velocity in each degree of freedom is also carried out using the NURBS basis functions. An implicit method is employed for time integration. The robustness and stability of this approach are studied taking into account a variation of the spatial and temporal refinement; various degrees of NURBS and time step sizes are considered. Finally, the results are compared with the standard isogeometric formulation.

- [1] M. Chasapi and S. Klinkel, A scaled boundary isogeometric formulation for the elasto-plastic analysis of solids in boundary representation, *Comput. Methods Appl. Mech. Engrg.* 333, 475-496 (2018)

Time-adaptive computations for the mortar finite element method

Matthias Grafenhorst (*TU Clausthal, Germany*)

10:10

Stefan Hartmann (*TU Clausthal, Germany*)

In recent years, mortar finite element methods have been successfully applied as space discretization scheme to a wide range of contact problems. The finite deformation contact formulation taken up is based on a mortar approach using so-called dual Lagrange multipliers. If the constitutive models of the material bodies are of rate-type, the entire system of equations represents a non-smooth system of differential-algebraic equations. This system will be investigated in connection with higher-order time integration methods using diagonally implicit Runge-Kutta methods for solving initial boundary value problems. As a preparatory step, we perform convergence studies in time for determining the time integrator behavior. This is done for 2D and 3D contact problems with and without friction. In a second investigation, we incorporate a time-adaptive step-size control based on local error estimations, which merely requires a small extra time-investment. Several numerical examples show the behavior of the proposed procedure.

S04.11 | Structural mechanics

Date: February 21, 2019
Room: SR 04

08:30-10:30

Model order reduction of a modular scale model of a high rise building

Nadine Walker (*University of Stuttgart, Germany*)
Peter Eberhard (*University of Stuttgart, Germany*)

08:30

This contribution deals with the numerical modeling of a physical scale model representing a high rise building that is to be built at the campus of the University of Stuttgart. The physical scale model is built at the Institute of System Dynamics of the University of Stuttgart. It consists of five structural units that are stacked. Each structural unit corresponds to one structural unit of the high rise building in its first planning version, where a structural unit is split into two storeys. Each structural unit consists of four pillars that support a floor panel. To brace the structure eight diagonal tie rods are used in each structural unit. The lowest structural unit is set up on a bottom plate. In the highest structural unit, the floor panel is replaced by a ceiling panel. This results in a modular setup of the scale model, consisting of five different components that are reused. The numerical modelling is done in a modular manner. To accelerate the simulation time model order reduction shall be performed on the model. Therefore, different model order reduction results are compared.

Numerical investigation of the movements of lapping particles

Raphael Bilz (*TU Kaiserslautern, Germany*)
Kristin de Payrebrune (*TU Kaiserslautern, Germany*)

08:50

Lapping is a machining process that improves technical surfaces before they are used in their final function. Smooth surfaces can be very important to avoid cracks in components exposed to high loads.

During lapping, the workpiece is placed on the lapping plate with a complex relative movement between both parts. In the gap between both parts, the lapping liquid with abrasive particles is placed. The moving particles can deform or cut the material of the workpiece, and iteratively smooth its surface. With appropriate operating parameters, as fluid and particle material, size and proportion, very high quality surfaces can be achieved.

To describe lapping processes, it is essential to understand the kinematics of the particles that influence the outcome of the manufacturing process, which can be accomplished by experiments and numerical studies. Here we will investigate the process numerically.

Using a discrete element method, we analyze the motion of complex shaped particles for varying conditions, such as different relative velocities and normal pressures and varying particle geometries.

We expect that the results will help to extend the knowledge of the underlying physics in the lapping process so that we can adapt it to specific requirements.

Effects of a temperature cycle on a rotating shrink fit with FGM-hub

Eray Arslan (*TU Wien, Austria*)

09:10

Tunc Apatay (*Gazi University, Turkey*)

Werner Mack (*TU Wien, Austria*)

In recent years, functionally graded materials (FGMs) have found increasing interest. Not only metal/ceramic- but also metal/metal-composites find more and more attention. For example, a steel/aluminum-FGM often allows for a substantial reduction of weight while exhibiting satisfactory strength; a usual production method is based on mixing a steel/aluminum powder appropriately, followed by cold pressing and sintering.

Hence, applying such an FGM also for shrink fits has been proposed recently. If a homogeneous steel inclusion is combined with a hub which is graded from pure steel at its inner surface to a steel-aluminum alloy or to pure aluminum at its outer surface, the performance of the shrink fit proves advantageous if it is subject to rotation. This is caused by the less decreasing interface pressure with increasing angular speed as compared to a steel-hub, accompanied by a substantial weight-reduction.

Indeed, for prescribed geometry and given friction at the inclusion/hub-interface merely the interface pressure determines the maximum transferable load. Hence, not only measures to increase the initial interface pressure have been an important subject in shrink fit investigations but also the question for the behavior under operating conditions. In particular, the occurrence of elevated temperature may influence the interface pressure considerably. Depending on the type of the temperature field, both a transient reduction and in case of partial plasticization also a permanent reduction of the interface pressure may occur.

Whereas - at least for elastic behavior - a spatially constant temperature rise does not influence the stresses in a homogeneous shrink fit, this is different in a shrink fit with FGM-hub. There, due to the unequal thermal properties of the FGM-constituents, even homogeneously elevated temperature will affect the stress distribution.

Hence, it is the aim of the present contribution to study the behavior of a rotating shrink fit with annular inclusion and power-law FGM-hub both for homogeneous and inhomogeneous heating. Presupposing slow temperature changes and thus quasi-steady temperature fields and a state of generalized plane strain, the problem can be treated analytically. It is shown that for an internally heated FGM-shrink fit the interface pressure even increases, and that, considering the interface pressure in relation to weight, using an FGM-hub generally may be beneficial.

Investigation of elastic grinding pins

Frederik Lamping (*TU Kaiserslautern, Germany*)

09:30

Kristin de Payrebrune (*TU Kaiserslautern, Germany*)

In some cases it is possible to reduce friction by using structured surfaces instead of polished surfaces. This is shown on the example of vehicle timing chain drives by Rosenkranz et al. [1]. The authors reduce friction of the chain drive by using cross-like structured chain links.

Whereas Rosenkranz et al. use a laser to produce the structure, this work investigates the usage of elastic grinding pins with silicone as base material. These grinding pins adjust to the chain links barrel-shaped geometry and lead to a structure perpendicular to the direction of rotation.

In a first step, different shapes and methods of adding the grinding material were analyzed. Further investigation on an improved test-bench were carried out with the most promising shapes - truncated cone and spheroid.

The aim of the investigation was to find the criteria for an optimal grinding surface appearance. Therefore, the elasticity of the base material and the particle size of the grinding material were varied. All tests were executed on acrylic glas tubes and the results verified with steel tubes. To come to a conclusion, the roughness profiles along the circumference at three positions of every specimen were analyzed.

Furthermore, tests with special grinding pins were executed. Instead of silicone as base material, these pins use a balloon filled with a magnetorheological fluid. By variing the magnetic field around these pins, it is possible to vary the viscosity of the fluid. As a result the contact pressure changes which effects the result of grinding.

[1] Rosenkranz, A., et al.: Tribological performance of laser-patterned chain links-Influence of pattern geometry and periodicity, *Wear* 370 (2017): 51-58.

Development of a simulation model for the automatic optimization of tools for multi-dimensional tube forming

Ralf Derr (*Saarland University, Germany*)

09:50

Anne Jung (*Saarland University, Germany*)

Stefan Diebels (*Saarland University, Germany*)

Requirements of tube forming processes in manufacturing of exhaust components such as light-weight construction and thus an error-free formability has increased in last years. Many experimental forming cycles are necessary to determine suitable setting parameters to meet the requirements. Finite Element (FE) models are used to represent the tube forming processes numerically and thus to reduce the number of experimental processes by simulations.

The aim of this study is the development of a software tool for the simulation of multi-dimensional tube forming processes by tube bending and tube embossing. Therefore, a self-developed graphical user interface was applied to build-up and simulate the tube forming processes. The material parameters for the FE model were determined by means of tensile tests. The validation of the simulation results was carried out by comparisons with the experimental results. Based on the obtained results using the FE method, an automated parameter optimization of the setting parameters was implemented to determine the optimal forming configuration.

The comparison with the experiments showed deviations in the result values of less than one percent. In addition to the numerical approximation, batch tolerances could also be identified as the source of the deviations. Furthermore, experimental forming errors could be numerically reproduced and corrected by modifying the parameter settings. The crucial influencing variables were determined by varying the parameter settings and a database for optimizing the tools was created. Based on user- defined requirements for the final tube geometry, suitable forming parameters could be determined by the optimization.

S04.12 | Structural mechanics

Date: February 21, 2019

14:00-16:00

Room: Audimax

A proper symplectic decomposition for inelastic shells

An Danh Nguyen (*RWTH Aachen University, Germany*)

14:00

Duy Thanh Truong (*University of Rostock, Germany*)

Bernd Markert (*RWTH Aachen University, Germany*)

We study a proper symplectic decomposition methodology to analyse the dynamics of shell structures by using the symplectic Brezis-Ekeland-Nayroles variational principle. For that purpose, a generalised Hamilton equation for the inelastic shells is first established. The efficient solution of the transient problem is then investigated by considering space-time separated representation. The symplectic model order reduction with greedy generation of a \mathbb{J}_{2n} -symplectic basis is used to set up an initial basis for accurate and stable results. The performance of the proposed numerical approach is illustrated through an example of a thin plate subjected to the shock wave loading.

Towards the incorporation of damage into solid-shells based on reduced integration

Oliver Barfusz (*RWTH Aachen University, Germany*)

14:20

Tim Brepols (*RWTH Aachen University, Germany*)

Jan Frischkorn (*RWTH Aachen University, Germany*)

Stefanie Reese (*RWTH Aachen University, Germany*)

Some years ago, a family of continuum finite elements based on reduced integration [1], [2], [3], [4] was investigated. Many structural components with different kinds of elastic and inelastic material behaviour were considered and these elements showed accurate results while being more efficient than similar three-dimensional formulations based on full integration. The objective of the present contribution is to extend the analysis to damage and fracture. To this end we present the incorporation of a gradient-enhanced damage model [5] into the framework of solid-shells based on reduced integration. Aspects on stability as well as the implementation in analogy to fully-coupled thermomechanical problems are discussed within the talk. Numerical benchmark problems reveal the capability and accuracy of the proposed framework.

References

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- [2] Reese, S. (2007). A large deformation solid-shell concept based on reduced integration with hourglass stabilization. *International Journal for Numerical Methods in Engineering*, 69(8), 1671-1716.
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On boundary conditions and constraints for representative volume elements of a two-scale shell formulation

Jan Zoller (*Technische Universität Darmstadt, Germany*)

14:40

Friedrich Gruttmann (*Technische Universität Darmstadt, Germany*)

In this contribution a coupled two-scale shell model is presented based on the algorithm in [1] which applies the concept of the FE²-method. The representative volume element (RVE) is meshed with solid elements. In the RVE edge effects can be reduced or even avoided by using periodic boundary conditions. However, this requires proper constraint to prevent rigid body movements. For this purpose, the theory in [2] for beams, which considers the shape of normal stresses over the cross section due to inhomogeneities of the material, is transferred to the shell problem. This procedure assumes geometrical and physical linearity. Furthermore, the RVE reacts to shear deformations not only with shear stresses but also with bending stresses. This leads to a vanishing shear stiffness with an increase of the freely selectable in plane size. This dependence of the shear stiffness is eliminated by another constraint on the normal stresses. Both constraints are incorporated using the method of Lagrange multipliers.

[1] Gruttmann, F., Wagner, W.: A coupled two-scale shell model with applications to layered structures. *International Journal for Numerical Methods in Engineering* 94(13) (2013), p. 1233-1254.

[2] Klarmann, S. C.: Geometrisch und physikalisch nichtlineare Mehrskalenmodellierung räumlicher Stabtragwerke. Darmstadt 2018

Coulomb dry friction contact in a non-material shell finite element model for axially moving endless steel belts

Jakob Scheidl (*TU Wien, Austria*)

15:00

Yury Vetyukov (*TU Wien, Austria*)

Both the penalty approach and the method of Lagrange multipliers are well established strategies for treating dry friction contact between deformable bodies in a finite element framework. While simple to implement, penalizing terms induce ill-conditioning in the system of equations and enforce the contact conditions only approximately. The method of Lagrange multipliers does not exhibit these drawbacks, but, when realised in its classical form, introduces additional unknowns and leads to unsymmetric matrices. Hence, it is usually implemented in an augmentation procedure, that adapts the penalty method to solve for the exact Lagrange multipliers iteratively. It is worth noting, that the treatment of normal contact with Lagrange multipliers does not converge for classical unshearable structural theories in a particular setting with concentrated contact interactions.

We illustrate the inherent difficulties one encounters, when trying to develop fast and reliable implementations of Coulomb's dry friction law, using a simple planar benchmark problem. Explicit algorithms are not robust and rely on small time increments to reach convergence. Implicit methods show improved stability and are less dependent on time step size.

We have developed a mixed, quasistatic Eulerian-Lagrangian shell finite element model for simulation of an axially moving, endless steel belt mounted on two cylindrical drums. The mixed kinematic description involves a change of variables between material and spatial coordinates. Concerning three-dimensional axially moving shells, the material coordinate in direction of the contour motion is replaced by a spatial one, while the transverse deflections remain in material description. The rotary motion of the pulleys and the axial movement of the belt are transmitted through dry friction behaviour in the contact regions. In this regard, equations of the Coulomb friction law need to be adjusted according to the mixed finite element kinematics. The

here presented penalty type of friction contact formulation is easily extendable to an augmented Lagrangian multiplier method.

Structural mechanics of endovascular stent grafts

Alexander Popp (*University of the Bundeswehr Munich, Germany*)

15:20

Ivo Steinbrecher (*University of the Bundeswehr Munich, Germany*)

Christoph Meier (*Technical University of Munich, Germany*)

Endovascular aortic repair (EVAR) has become a very successful minimally invasive procedure in vascular surgery for supporting abdominal aortic aneurysms (AAA) that are at risk of rupture. As main structural component, EVAR involves so-called stent grafts composed of slender metal stent wires and a thin-walled synthetic graft fabric. The modeling and computational analysis of stent grafts poses several serious challenges: reduced-dimensional modeling using novel nonlinear beam and shell formulations, nonlinear material behavior, structural stability, finite element discretization techniques as well as bonded and unilateral contact modeling. Besides the mechanical perspective, we will also highlight the complexities that arise due to the complex geometries of marketed stent grafts, which typically include complex stent wire patterns, sutures between wire and encasing fabric, bifurcations and special leg insertions. Mostly bare-metal stents have been considered in the literature so far, starting from very simple ideas and gradually improving those towards parametrized high-fidelity models based on micro-CT scans of the device. Finite element models of stent grafts, i.e. models that explicitly consider the encasing fabric, have only become accessible to computational analysis in recent years. However, almost all contributions available today employ a solid-based approach, i.e. a finite element discretization of the stent wires as a 3D solid body using volume elements. Considering that stent wire diameters are typically much smaller than the device length scales, reduced-dimensional structural modeling based on nonlinear beam theories appears as a promising alternative. The same holds true for the encasing fabric, for which cutting-edge shell models could be explored. Within this contribution, we will present recent advancements in the robust and efficient structural modeling of stent grafts. Specifically, geometrically exact beam finite element formulations based on the Kirchhoff-Love theory will be reviewed and their extension towards stent graft applications will be highlighted. While most existing beam elements are of Simo-Reissner type, the novel formulations focus on highly slender rod-like components (such as stent wires), where they allow for dramatic computational efficiency gains. In terms of contact interaction, a new unified framework for beam-to-beam and beam-to-solid contact will be presented, which transfers findings from 3D solid contact formulations and mortar finite element methods to the new structural models. Several numerical examples will demonstrate the applicability of our methods to the different stages of stent graft placement. This includes crimping into the delivery catheter, unfolding of the device, placement into idealized arteries as well as typical bending motions.

Impact of thin walled square aluminum tubes

Nima Jafarzadeh Aghdam (*RWTH-Aachen University, Germany*)

15:40

Uday Bhaskara Chary Tatikonda (*University of Duisburg-Essen, Germany*)

Jannik Bühring (*RWTH-Aachen University, Germany*)

Narasimha Rao Mekala (*RWTH-Aachen University, Germany*)

Kai-Uwe Schröder (*RWTH-Aachen University, Germany*)

From early stages of automotive industry passenger safety and crashworthiness of the car have gained high attention. Cars are becoming faster and they require more efficient crash structure. Besides, light weight strategies are inseparable from new structure designs. Thin-walled profiles are widely used as crash absorbers. In this paper square thin walled structures under impact

load is studied numerically. Crash boxes are made by aluminum. Mechanical properties of the material are extracted experimentally. ABAQUS commercial software is used for simulating the crash box. Simulated model is validated experimentally using drop tower test.

High energy absorption of a crash box is a desired goal of a robust crash box. Folding pattern of the structure has significant effect on energy absorption of it. In this study effects of different parameters such as wall thickness and width on behavior of the crash box under impact load have been investigated. It has been shown even though width increase results in higher energy absorption, specific energy absorption of the crash box is decreased.

S04.13 | Structural mechanics

Date: February 21, 2019

14:00-16:00

Room: SR 04

Specimen design for extreme uniaxial tension-compression tests of rubber materials

Lars Kanzenbach (*TU Chemnitz, Germany*)

14:00

Jörn Ihlemann (*TU Chemnitz, Germany*)

For material characterization and model parameter identification different types of specimens are required. Particularly, the uniaxial compression domain plays an import role in many technical applications. For this, a specimen-setup is developed, which enables compression up to a strain of -40 % and tension up to 300 % [1]. Thereby, a nearly homogeneous deformation field is still preserved. In this contribution the specimen-setup is optimized and extended for extreme uniaxial compression tests up to a compression strain of -70 %. The principal idea for developing a new specimen-setup (via eigenfrequencies as a measure for instability) can be seen in a previous publication [2]. For extreme compression tests the calculation of the test-setup is extended. Furthermore, a new measurement strategy, which enables the investigation of strains at such extreme compression levels, is introduced. The developed specimen-setup is realized and tested. The tests were performed with filled natural rubber and filled EPDM. Note, that for such extreme compression tests the measuring zone is very limited. Hence, requirements concerning the measuring device increase. For this, an aiming kit and a DIC measuring system was used. Furthermore, the measuring system enables the measurement of the horizontal displacement of the center point of the test specimen. It is important to know, that even for such extreme compression tests no buckling occurs.

The optimized and extended specimen-setup enables extreme uniaxial tension-compression tests up to a compression strain of -70 %. Finally, phenomenological characteristics of rubber, like Payne effect, Mullins effect, permanent set, relaxation and creep can be investigated at such extreme compression levels.

Acknowledgements

The authors gratefully acknowledge the financial support from Vibracoustic GmbH & Co. KG and FTI SE & Co. KG.

References

- [1] Kanzenbach, L., Naumann, C. and Ihlemann, J. (2016), Specimen design for high precision tension-compression tests. *Proc. Appl. Math. Mech.*, 16: 207-208. doi:10.1002/pamm.201610092
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DIC-measurement and its approach for the FEM-simulation of "Die-Less-Hydroforming"

Andreas Metzger (*Karlsruhe Institute of Technology - KIT, Germany*)

14:20

Daniel C. Ruff (*Karlsruhe Institute of Technology - KIT, Germany*)

Thomas Ummenhofer (*Karlsruhe Institute of Technology - KIT, Germany*)

Digital Image Correlation (DIC) - measurement is a non-contact optical measurement method, which is currently very popular in the context of experimental investigations. For this, the test specimens are provided with a speckle pattern on their surface. At least two or more cameras, whose test field has been calibrated in advance, are used for continuous image acquisition during the specific experimental test. Afterwards a spatial model of the specimen configuration that can be used for further evaluation is calculated by software on the basis of this image data.

Within "Die-Less-Hydroforming", an increasing innovative forming technology, see [1] and [2], the DIC-measurement may be used for two tasks at once:

By using the DIC-measurement during the tensile test of the initial steel sheet material used for the double-layered "Die-Less-Hydroforming"-blank, it is possible to measure continuously the true cross-sectional area at the beginning of necking and almost to the end of the test. Due to the availability of this information, it is possible to determine a true stress - true plastic strain - curve. This curve is also known as flow plot, which with conventional testing methods, especially for the case of flat tensile test specimen, cannot be determined up to such a late loading state. Often it is only estimated by mathematical approximations based on standard tensile test performance. For the FEM-forming-simulation of "Die-Less-Hydroforming", however, such a real flow curve is required.

Furthermore, within the framework of the classical application of a DIC-measurement, the forming process of "Die-Less-Hydroforming" can be investigated continuously during the experiment. This including change of geometry and surface strains.

Consequently, in the present paper, both described DIC-measurement applications are used in the context of FEM-simulations of "Die-Less-Hydroforming". In detail, the determined flow curve is used as input for the material parameters in the simulation and the DIC-measurement during the "Die-Less-Hydroforming" process is used for the validation of the calculated 3D-shape and the corresponding stress and strain states. This approach is demonstrated by selected "Die-Less-Hydroforming"-samples.

References:

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[2] Metzger, A., Ruff, D.C. and Ummenhofer, T. (2015): Investigations on clamping effects with "Die-Less-Hydroforming-Structures", Proc.Appl.Math.Mech.15, 215-216, doi:10.1002/pamm.201510098

Experiments on wave propagation in soft resins

Sam Aghayan (*Siegen University, Germany*)

14:40

Sören Bieler (*Siegen University, Germany*)

Thomas Reppel (*Siegen University, Germany*)

Kerstin Weinberg (*Siegen University, Germany*)

The investigation of the wave propagation in soft materials is essential, as it would help to study the effects of shock waves, particularly in the impact. In this study, a Split Hopkinson Bar (SHB) setup is utilized in order to induce a wave by applying dynamic impact. Different types of resin based materials, used as 3D printer materials, are selected to investigate the wave

propagation. The chosen resins are elastomers and thermoplastic materials, mostly having soft materials behavior. The specimens were manufactured by 3D printing in a cylindrical shape. It should be noticed that this particular study is basically part of a larger project, concerning over applying the same procedure to investigate the behavior of soft biological tissue, under the impact in SHB test.

The test would be done in two different bar set ups, in which the first set of tests is done with aluminum bars and the second set is carried out by polymer bars in order to study the effect of the bar materials on the tested resins.

The principal assumptions and the role of pulse shaping, as an approach to achieve constant strain rates and dispersion reduction, are discussed. Moreover, in parallel to the experiment finite element simulations of SHB test are performed. The measured dynamic elastic modulus and the stress-strain behavior of the tested materials are presented.

Comparison of structured and conforming meshes in FE analyses of textile reinforced air spring bellows

Nina Heinrich (*TU Chemnitz, Germany*)

15:00

Jörn Ihlemann (*TU Chemnitz, Germany*)

The bellows as the central part of air springs contains a certain number of reinforcing textile cord layers embedded in a rubber matrix. Typically, such cords are a twisted structure made from multi-filament yarns. Thus, air spring bellows represent a composite component that is characterized by both highly complex geometry and strong nonlinear material behavior of its constituents. This contribution aims at comparing two different approaches of how these challenges can be addressed in the framework of finite element analyses.

The test model is inspired from cylindrical, sleeve-type air springs. These are considered as cyclic symmetric so that modelling can be narrowed down to a single straight slice. A pressure load is applied onto the inner surface while the top and bottom surface of the slice are clamped. Isotropic hyperelastic material behavior is assigned to the rubber matrix whereas the cords are equipped with a transversely isotropic hyperelasticity that is capable of taking the local filament direction into account.

A simple, straight forward approach for the discretization of the slice is to generate a structured hex mesh that initially disregards material interfaces. Instead, by means of a geometry model for the cords, material areas are distinguished at integration point level, which implies that different materials may be present in one element. The other, more traditional approach is to generate a conforming mesh in which material interfaces coincide with element faces. Due to the complex geometry, this meshing strategy requires much more effort but, on the other hand, it ensures smooth material interfaces.

For the test model, both discretization approaches are implemented and investigated in a convergence study. Results concerning performance, global quantities like diameter, and local measures such as strain distribution will be presented.

Modal flatness analysis of thin sheets

Peter G. Gruber (*Linz Center of Mechatronics, Austria*)

15:20

In the industrial process under investigation, sheets of material are produced and reduced in their thickness as they pass a sequence of successive interface devices.

Caused by improper settings or various disturbing control actions the finalized sheets may exhibit residual stresses, and thus flatness defects. Typical defects in the process under investigation are longitudinal edge and center buckles. If one could measure the stress distribution at the sheets, the particular defects could be anticipated by a controller. However, the rough environment does

not allow any stress measurements, whence there is no way to prevent the sheets from buckling. As a remedy wave buckles are scanned with visual devices on a single line orthogonal to the transport direction.

The two dimensional field of wave buckles may thus be approximated by a time sequence of line scans. The aim of our investigations is to complement those measurements with modal analysis by a simulation model, and to use this information for developing an efficient surrogate model with which a controller may operate on the plant.

On the macro to micro transformation

Momme Jahn (*Helmut Schmidt Universität, Germany*)

15:40

Martin Meywerk (*Helmut Schmidt Universität, Germany*)

The investigation of solids with large displacement and fractures is a challenging task. Such problems could occur in the study of tyre-soil interactions. Some of these problems have the peculiarity that the treated soil domain is very large in comparison to the contact-surface or the wheel tracks.

A capable method to investigate huge displacements and fractures in soils is the Discrete-Element-Method (DEM). The drawback of this method is the huge computational effort which increases with an increasing number of elements.

An alternative way to study solids is the Finite-Element-Method (FEM). The benefit of this method is the lower computational effort for large domains in comparison with the DEM, but the drawback is the high effort to investigate huge displacements or fractures.

If the benefits of both methods should be used, a transformation from FEM to DEM and vice versa must be defined.

This enables the possibility to investigate the soil in the initial stage with the FEM. If huge displacements occur, since the tyre deforms the soil, the affected Finite-Elements should be transformed to an assembly of Discrete-Elements. If this domain is unloaded again, since the tyre passed this location, the transformation from DEM to FEM could be performed. Thus only the region where currently huge displacements occur is modeled with DEM while the rest is investigated with FEM.

The transformation from DEM to FEM could be performed with homogenization techniques, which is a subject of research since many years.

The transformation from FEM to DEM isn't investigated a lot.

The goal of this transformation is to create a particle assembly which has equivalent mechanical attributes like the corresponding FEM region, which is treated with the Cosserat-continuum.

A prerequisite is the definition of a dual cell system where a unique integration territory is defined for each particle and for each particle-contact.

The mechanical attributes, which should be preserved, are the mass, the moment, the moment of momentum, the kinetic energy, the stress energy and the energy of stress-moments. In this presentation the transformation of these mechanical quantities from FEM to DEM is investigated.

S04.14 | Structural mechanics

Date: February 21, 2019

17:40-18:40

Room: Audimax

Soil mechanical influence on numerical goundation design of tower cranes

Herbert W. Müllner (*PORR Design & Engineering GmbH, Austria*)

17:40

Herbert R. Meister (*PORR Design & Engineering GmbH, Austria*)

The static design of foundations for tower cranes is mostly based on calculations of structural safety like tilting, sliding and groundbreaking. Nevertheless further investigations considering the interaction between soil and structure including settlement calculations for evaluating inclination of the crane, which is restricted by the suppliers of tower cranes [1], are essential for safe and economic foundation solutions.

Mainly depending on the locality of the building site a distinction is drawn between cranes using undercarriage or foundation cross and cranes using base anchor bolts which are set directly in a concrete foundation. Nearby temporary construction pit systems using diaphragm walls, soldier pile walls or bored pile walls highly affect the static design of crane foundations, too. In addition, soil investigation reports often do not include all required soil parameters, stiffness modulus and bedding factors, respectively.

Based on the experience of more than 140 tower crane positions throughout Europe a method has been developed satisfying the normative and crane specifically requirements and meeting the standards of one of the biggest building contractors in Europe.

In this contribution the method and its application is presented. Using singularity functions [2] a reinforced concrete design is performed under consideration of a stiff foundation. In order to fulfill the settlement limits [1] a finite element numerical analysis is done. A back calculation of the required bedding factor using the vertical displacements and the soil parameters completes the analysis.

The higher effort in the static design of foundations allows the application for both, standard and problematic crane foundations. The latter are asymmetric and separated foundations as well as combination with deep foundations and temporary construction pit systems, respectively.

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Dealing with stochasticity in seismic safety analysis

Christian Gasser (*TU Wien, Austria*)

18:00

Christian Bucher (*TU Wien, Austria*)

Earthquakes are highly stochastic processes. As a consequence, the variability of the response of a structure subjected to different ground motions with same intensity is very high. This fact can vividly be seen in a response spectrum showing the responses of a SDOF oscillator to a set of earthquakes which are expected in a location with a defined return period. In engineering practice, it is common to deal with these uncertainties by using design spectra, which are smoothed curves based on quantile values of a number of SDOF responses. The strength of the method is its straightforward applicability. However, the assessment of structural response is very simplified since it relies on some superposition of spectral responses of a linear system. As a matter of fact, a realistic simulation of the (ultimate) behaviour of a structure

has to be based on a time history analysis. In this way, nonlinearities may be accounted for, especially material behaviour beyond linear elasticity, including the dissipative effects of ductile components, which are of high relevance in earthquake engineering. The variability of ground motions can then only be considered by performing a Monte Carlo simulation with different ground motions (which might be either scaled records or artificially generated ground motions). However, the task becomes more expensive than Monte Carlo simulation is anyhow since, in principle, damage (resp. failure) probabilities have to be estimated for each intensity level. Eventually, fragility curves for different limit states are obtained, i.e. exceedance probabilities conditional on the ground motion intensity level.

This contribution primarily focuses on methods to reduce the computational effort of the Monte Carlo simulations. Specifically, in a first approach, the fragility curves are obtained by fitting lognormal curves to binary (failure / no failure) outcomes of the simulation runs by means of the maximum likelihood method. In a second approach, the exceedance probabilities are estimated by means of a cloud analysis of the exact outcomes of the simulation results.

The methods are not only developed mathematically but they are applied on the model of an arch dam. The realistic modelling of the physical problem is an utmost important prerequisite for any further result evaluation. Hence, various damage scenarios are investigated in detail and failure is studied by a plastic-damage model for concrete.

A damage detection study of a bridge using bypassing vehicles and computational intelligence

Daniel Frank Hesser (*RWTH Aachen University, Germany*)

18:20

Franz Bamer (*RWTH Aachen University, Germany*)

Bernd Markert (*RWTH Aachen University, Germany*)

Structural integrity is an ubiquitous topic in research and daily living. Conventional monitoring strategies follow a preventive maintenance plan or require permanent installation of sensors. These steps are time and cost inefficient taking into account the number of bridges to be monitored. In this study, a bridge structure is monitored passively using the acceleration signal of a bypassing vehicle. Thereby, the signal is measured on the vehicle. The health status of the bridge can be evaluated after each pass, which allows a continuous monitoring of the structure. A numerical model of a bridge and bypassing car is carried out to prove the feasibility of this approach and to create a large database with different damage locations and vehicle velocities. Moreover, an artificial neural network is trained on that database to detect damaged bridge structures. The proposed method proves the feasibility of monitoring the structural integrity of bridges and supports conventional maintenance methods. Therefore, a combination of active and passive monitoring strategies pave the way to efficient and cheap infrastructure monitoring strategies.

S04.15 | Structural mechanics

Date: February 22, 2019

08:30-10:30

Room: Audimax

A first order homogenization approach for structural elements: beam kinematics

Simon Klarmann (*RWTH Aachen University, Germany*)

08:30

Friedrich Gruttmann (*TU Darmstadt, Germany*)

Sven Klinkel (*RWTH Aachen University, Germany*)

This contribution deals with a first order homogenization approach for structural elements with the focus on shear deformable beam elements. The homogenization theory itself is based on the well-known Hill-Mandel condition. Therefore, the numerical treatment leads to a coupled multiscale approach whose calculation can be performed with the so-called FE2 scheme. As a result, not only cross-sectional properties in the linear elastic case can be evaluated but also geometrical and physical nonlinearities can be considered. Since the mesoscale, which will be homogenized, is modelled by 3D brick elements, the considered global structure only needs to be periodic to allow a definition of a representative volume element (RVE). Thus, the procedure is not limited to pure cross-sectional modelling, but is also able to consider inhomogeneities in the longitudinal direction of the system.

As the beam kinematics do not describe the complete deformation gradient or strain tensor, the equilibrium condition introduces a length dependency of the homogenized shear stiffnesses and the stiffnesses which depend on them due to eccentricities. This is due to the fact that the averaged shear deformation of the RVE does not linearly depend on its length multiplied by the beam shear deformation. To overcome this problem, additional constraints are introduced which ensure this linear connection. They are chosen in a way that they do not contribute to the virtual internal work. Therefore, the Hill-Mandel condition is not affected by them. With these assumptions, the length dependency is eliminated and the averaged shear deformation of the RVE equals the shear deformation of the beam kinematics. As a result, the method is able to reproduce well-known cross-sectional values known from the literature and is also capable to evaluate complex nonlinear systems. For the latter, the agreement of the results with those of continuum models is very satisfying.

Evidences of the non-negligible effects of the orientation of material principal directions on the structural response of a planar anisotropic beam

Giuseppe Balduzzi (*TU Wien - Vienna University of Technology, Austria*)

08:50

Simone Morganti (*University of Pavia, Italy*)

Josef Füssl (*TU Wien - Vienna University of Technology, Austria*)

Mehdi Aminbaghai (*TU Wien - Vienna University of Technology, Austria*)

Alessandro Reali (*University of Pavia, Italy*)

Ferdinando Auricchio (*University of Pavia, Italy*)

Effective analysis and design of composite structures require beam and plate models capable to handle the material anisotropy. Nowadays the need of accurate analysis tools is even more urgent due to the fast development of additive manufacturing technologies, that allow to create structural elements with variable orientation of fibres or made of complex materials (e.g., metamaterials, lattice structures, ...), possibly making the material exhibit anisotropic behaviour and arbitrary orientation of material principal directions.

The present contribution aims at shedding light on the effects that the arbitrary orientation of material principal directions produce on the beam constitutive relations, stiffness, and displacements. Accordingly, we derive a planar linear-elastic beam model with enhanced constitutive relation assuming that the cross-section behaves as a rigid body. Thereafter, we compute the analytical solution for simple geometries, loads, and boundary conditions. Analytical results highlight that coupling terms relating transversal internal force with curvature (and bending moment with shear strain) do exist in anisotropic beam constitutive relations and significantly influence the response of the structural element. In fact, in addition to standard bending and shear contributions, a third addend (consequence of the non-vanishing coupling terms) affects the transversal displacement magnitude also for extremely high length versus thickness ratios, turning out to be more significant than shear contribution.

A systematic comparison with 2D finite element solutions, obtained using very fine meshes, demonstrates the effectiveness of the proposed modelling approach. Specifically, the computational cost of the proposed beam model is similar to the one relative to much simpler beam models, classically adopted engineering practice. Nevertheless, the proposed model estimates maximal displacements and internal forces with relative errors usually smaller than 2%, describing phenomena that occur in multilayer anisotropic beams with an accuracy reasonable and sufficient for most engineering applications. Conversely, coarse adaptations of beam models developed for isotropic structural elements may lead to errors greater than 15%, resulting inadequate also for basic engineering applications.

A higher-order shear deformation approach to the mixed-mode buckling problem in composite laminated beams

Siham Mittelstedt (*SOGETI High Tech GmbH, Germany*)

09:10

Christian Mittelstedt (*Technische Universität Darmstadt, Germany*)

This paper presents a semi-analytical method for the mixed-mode buckling problem in composite laminated beams. Mixed-mode buckling describes the interaction and the mutual influence between the local buckling modes of the segments of shear deformable composite laminated beams, i.e. the simultaneous local buckling of the web and the flanges of a beam, for instance with an I cross-section. The buckling analysis employs Reddy's third-order shear deformation theory for the local buckling behavior of flanges and webs of open-profile cross-sections where the laminates that constitute those segments may exhibit arbitrary but symmetric layups. The Ritz-method in conjunction with adequate series expansions for the buckling degrees of freedom is used wherein the webs and flanges are considered separately and later on unified by employing Lagrangian multipliers. The results are compared with the buckling loads as obtained by finite element computations, and a very satisfying agreement is found. The semi-analytical analysis method can be shown to be significantly more efficient in terms of the required computational effort when compared to purely numerical means of analysis.

Nonlinear finite element study of beams with elasto-plastic damage behavior in the post-buckling regime

Benjamin Werner (*TU Wien, Austria*)

09:30

Melanie Todt (*TU Wien, Austria*)

Heinz E. Pettermann (*TU Wien, Austria*)

Lattice materials can be described as arrangements of rigid-jointed beams. Loads on the macroscopic level of the lattice material can cause a loss of structural stability on the microscopic level and therefore, the buckling of beams. In this study the post-buckling behavior of beams with elasto-plastic material properties and ductile damage is investigated with the finite element

method to reveal the effect of progressing damage and localization on the post-buckling deformation. The aim is to find a proper discretization to predict damage and localization sufficiently accurate for varying buckling modes. At the same time it has to be computational inexpensive enough to investigate the macroscopic response. The macroscopic response is usually determined by analysing large sections of the lattice material and by modeling the microstructure explicitly. The present study also includes the investigation of the mesh dependency. To determine a proper discretization the beam element type, the number of elements, the number of section points, as well as the boundary conditions are varied in the numerical analyses. The results are compared to a reference solution from a simulation with a much finer discretization. The applied elasto-plastic material with ductile damage is characterized by perfect plasticity and a very early onset of damage. The damage leads to localization and a rapid decline of the reaction forces. The predicted deformations deviate from the initial eigenmode shapes with progressing damage and localization. Based on the presented results the macroscopic behavior of damaged lattice materials can be investigated in future studies.

Extension of Boley's method to two-layer rectangular beams

Johannes Gahleitner (*JKU Linz, Austria*)

09:50

Hans Irschik (*JKU Linz, Austria*)

A rectangular beam, composed of two firmly bonded layers having dissimilar linear elastic materials, is considered in a state of plane stress. In the present contribution, Boley's method, originally derived for single-layer beams, see Boley and Tolins[1], is extended to this two-layer case, in order to obtain solutions that do exactly satisfy the field relations of linear elasticity in each of the layers, the boundary conditions at the upper and lower surfaces of the beam, as well as the transition conditions at the interface of the two layers. Boley's original method [1] yields a fast convergent step-by-step improvement of the classical Bernoulli-Euler theory of beams, the first correction step dating back to v. Karman [2]. In each additional step, there appear derivatives of bending moment and normal force of an increased order. Via equilibrium relations, this allows to predict the number of steps with non-vanishing contributions. In [1], results of the first three steps were presented in illustrative Tables. In the present contribution, we succeed in presenting results for the composite two-layer beam that are in complete analogy to the single-layer Tables in [1] and thus can be used likewise. Particularly, we extend a method by Irschik [3] for single-layer beams, in which the results of Boley and Tolins [1] were re-written to formulate an enhancement of the fourth-order boundary value problem of the classical Bernoulli-Euler beam theory, involving fictitious eigenstrain-type loadings that can be taken directly from the Tables in [1]. Two approximate boundary conditions then can be assigned at each of the beam ends, so that bending moments and normal forces can be straight-forwardly computed also in case of redundant beams. Re-substitution into the Tables in [1] gives semi-exact solutions that coincide with various heuristically obtained semi-exact plane stress solutions for statically determinate beams from the literature, see e.g. [4]. In the present contribution, the systematic procedure derived in [3] for single-layer beams is extended and applied to a redundant two-layer beam.

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On a similarity transformation based on a Jordan Decomposition leading to an exact transfer matrix for a composite beam structure with refined Zigzag kinematics

Karin Nachbagauer (*University of Applied Sciences Upper Austria, Austria*)

10:10

Heinz Wimmer (*University of Applied Sciences Upper Austria, Austria*)

The Refined Zigzag Theory (RZT) is one of the most promising approaches for analysing composite structures today. Since its appearance many contributions have been published dealing with finite elements for laminated structures based on the efficient kinematic of RZT. For composite beam-columns C0-elements of different orders as well as p-type approximations have been formulated and utilized. The governing equations can be assembled in a first order differential system and could be solved by different numerical strategies, e.g., finite difference methods, Runge-Kutta methods or the transfer matrix method.

In this work a new approach for the analysis of laminated composite beams will be presented which can be considered as exact. The first order differential system is solved here by following two parallel approaches in establishing the transfer matrix: a series solution and a similarity transformation.

The proposed similarity transformation is based on a Jordan Decomposition using the eigensystem of the system matrix and leads to an explicit and analytical form of the transfer matrix for the static and dynamic case. Therefore With the well-known relations between the transfer- and the stiffness matrix an exact version of the latter one can be obtained. As a further advantage, this procedure provides the exact values of the first derivatives of the essential kinematic variables, which are used to calculate the strains and stresses in the laminate.

S05 | Nonlinear oscillations

Organiser: Katrin Ellermann (*Graz University of Technology, Austria*)
Leo Dostal (*Hamburg University of Technology, Germany*)

S05.01 | Nonlinear oscillations

Date: February 19, 2019
Room: HS 16

08:30-10:30

From cybernetics to mechatronics - seven decades of interdisciplinary engineering

Werner Schiehlen (*University Stuttgart, Germany*)

08:30

Cybernetics is an interdisciplinary approach for exploring controlled systems. Norbert Wiener defined cybernetics in 1948 as "the scientific study of control and communication in the animal and the machine".

Cybernetics is applicable when a system being analyzed incorporates a closed feedback loop where action by the system generates some change in its environment and that change is reflected in the system in some manner that triggers a system change. Cybernetics is relevant to, for example, mechanical, physical, biological, cognitive, and social systems.

Engineering cybernetics established 1954 by H. S. Tsien is a field of cybernetics, which deals with the question of control engineering of mechanical systems as well as chemical or biological systems. It is used to control and predict the behavior of such a system.

Mechatronics unites the principles of mechanics, electronics, and computing to generate a simpler, more economical and reliable system. An industrial robot is a prime example of a mechatronic system, it includes aspects of mechanics, electronics and computing to do its day-to-day jobs.

The word "mechatronics" originated in Japanese-English and was created by Tetsuro Mori, an engineer of Yaskawa Electric Corporation in 1969. Nowadays, the word is translated in each language and the word is considered as an essential term for industry.

Due to actively controlled elements in gyroscopic systems various effects may occur as presented 1980 by Kurt Magnus. For their examination quite general equations of motion are derived, which allow some global statements concerning the stability of gyro-systems with motor-driven rotors. Furthermore, it is shown that unstable behavior with respect to the attitude angles is possible due to effects of kinetic drift.

The control design leads also to new operational machine parts like the suspensions of magnetically levitated vehicles defined 1984 by Eveline Gottzein as magnetic wheels. The close connection between analytical robotics and mechatronics was highlighted in 1995 by Wolfram Stadler.

The high reputation of mechatronics as a science was recently underlined by a mark of distinction for Kurt Magnus by a commemorative plaque erected from the foundation Stiftung-Werner-von-Siemens-Ring and unveiled at the Technical University of Munich on July 19, 2018.

The Stiftung Werner-von-Siemens-Ring honored the scientific work of Kurt Magnus with respect to GYROSCOPES and VIBRATIONS as well as CO-FOUNDER OF MECHATRONICS including nonlinear oscillations, too.

Thus, from the early contribution of Norbert Wiener in 1948 to the recognition of the service of Kurt Magnus it took seven decades.

Sensitivity in machining systems

Peter Eberhard (*University of Stuttgart, Germany*)

09:10

Dominik Hamann (*University of Stuttgart, Germany*)

Machining is important for many manufacturing processes and raises many challenging questions in research. In stability analysis, time-periodic delay-differential equations are used for the modeling of the regenerative effect. Designing machining processes, frequently high computational effort occurs for providing stable operating points in so-called stability lobe diagrams.

Especially for thin-walled workpieces, varying workpiece dynamics has to be considered due to position dependency of the tool as well as material removal. Furthermore, simplifications in modeling and difficulties in identifying parameters affect availability of robustly stable operating points. According to this, enhanced stability lobe diagrams are important, including information about the effects on the stability limit and sensitivity of the systems. Enhanced stability lobe diagrams can support engineers in selecting robustly stable and efficient operating points as well as researchers in acquiring insight into the system behavior.

Chatter stability analysis for milling processes

Roman Binder (*Fill Gesellschaft m.b.H, Austria*)

09:30

Katrin Ellermann (*Graz University of Technology, Austria*)

Harald Sehrschrön (*Fill Gesellschaft m.b.H, Austria*)

Machine tools are some of the most important components in modern production engineering. Therefore, they are essential for cost-effective workpiece production. However, full utilization of the available cutting performance is often inhibited by chatter vibrations, which can lead to poor surfaces, reduced tool life, increased noise emissions and even damage to the machine. Stability charts in which the maximum depth of cut is plotted as a function of the spindle speed are well-established. Additionally, these stability charts are also a useful tool for evaluating machine structures during the design process.

The stability of machining processes can be determined by experimental tests as well as by simulations. The corresponding mathematical models are nonlinear, non-homogeneous, delay-differential systems with time-periodic coefficients. Several methods either in frequency domain or in time domain exist to solve the resulting equations approximately.

The aim of this work is the experimental and simulative determination of a machine tool's dynamic behaviour. The structural behaviour of the machine tool is obtained by means of standard modal testing. Based on the measured results, the stability of machining processes is investigated with a particular focus on regenerative chatter and its causes. In order to achieve this, several methods for generating stability charts are implemented which are either based on simplified modal models of the machine tool for standalone simulations in Matlab®[®], or on an integrated simulation in the multibody simulation software RecurDyn®[®].

The determined frequency response functions display clear resonance peaks of the machine, which vary with the axis position. From this, modal models with few degrees of freedom could be generated. A time domain simulation using the Matlab®[®] ode23-Solver and a stability criterion based on periodic orbit sections is compared to the analytical solution of a Zero Order Approximation (ZOA) in frequency domain and a Full Discretization Method (FDM) in time domain. The influence of various parameters on the stability is investigated. The implemented simulation methods for calculating the stability behaviour are found to compare well with the results of literature and thus can be used for evaluating machine structures during the design process in the future.

Nonlinear dynamical systems excited by large amplitude random loads

Leo Dostal (*Hamburg University of Technology, Germany*)

09:50

The presented research deals with methods for the study of complex interactions between noise and nonlinearities in dynamical systems. Practical applications of this research are beginning to appear across the spectrum of mechanics; for example vibration absorbers, ship dynamics, energy harvesting.

In the presented approach perturbed Hamiltonian systems are considered, which are damped and excited by an absolutely regular large amplitude non-white Gaussian process. Analytical and semi-analytical solutions to the corresponding nonlinear stochastic differential equations are determined. The approach is based on a limit theorem by Khashminskii, from which a class of methods has been derived known as stochastic averaging. In the presented approach Homoclinic orbits, which divide the phase space of the corresponding Hamiltonian flow into different regions, are mapped to a graph in the one degree of freedom case. For two degree of freedom systems this procedure results in a mapping to a book, and so on for higher degrees of freedom. From the drift and diffusion of the resulting averaged process, probability density functions and first passage times are obtained.

An experimental setup for such dynamical systems is presented as well, including results for the case of large amplitude random excitations.

Vibrations of an alpine ski under structural randomness

Robert Eberle (*University of Innsbruck, Austria*)

10:10

Michael Oberguggenberger (*University of Innsbruck, Austria*)

In alpine skiing the vibrations of the skis influence the performance of a skier considerably. A ski can be modelled as an Euler-Bernoulli beam, where the vibrations can be described by the equation of motion of a damped Euler-Bernoulli beam

$$(EI(x)w_{xx})_{xx} + \rho A(x)w_{tt} + \beta(EI(x)(w_t)_{xx})_{xx} + \alpha \rho A(x)w_t = f. \quad (1)$$

Here, x denotes the longitudinal coordinate, t the time, $EI(x)$ the flexural stiffness, $w(x, t)$ the deflection of the ski in vertical direction, ρ the mass density, $A(x)$ the cross sectional area of the beam, and f the line forces acting on the ski. The coefficients β and α stand for the damping coefficients. The main characterisation of a ski is its bending stiffness $EI(x)$, which can be measured in the lab. A ski is a composite material that consists of different layers, which are glued together. Consequently, measurements show variations in the bending stiffness $EI(x)$. These variations can be considered by adding a random field $r(x, \Theta)$ to the mean bending stiffness $EI(x)$ in the beam equation (1)

$$EI(x, \Theta) = EI(x) + r(x, \Theta) \quad (2)$$

We investigated the vibrations of a ski in the following situation. The ski was clamped in the centre, the ski tip was deflected and released. This experiment accords with the vibration of a deflected cantilever beam and was modelled by equation (1) with boundary conditions (clamped - free)

$$w(0, t) = 0, w(x, t)_{xx} = 0 = 0$$

$$w(x, t)_{xx=L} = 0, w(x, t)_{xxx=L} = 0$$

and initial deflection and velocity:

$$w(x, 0) = w_0(x)$$

$$w(x, t)_{t=0} = 0$$

The initial deflection $w_0(x)$ was calculated by the static beam equation. The differential equation was solved by the spectral method. After a Monte-Carlo simulation the eigenmodes and eigenfrequencies were determined and analysed. In the future, the presented approach will be applied on other structural problems, as for example the vibrations of a composite bridge under traffic load.

S05.02 | Nonlinear oscillations

Date: February 19, 2019

16:30-18:30

Room: SR 06

Influence of friction on the locomotion of soft robots

Kristin de Payrebrune (*TU Kaiserslautern, Germany*)

16:30

The recent interest in soft robots results from their adaptability, versatility and flexibility, which is very advantageous for new applications in human-robot interaction, health care or field exploration. Many feasibility studies have already demonstrated the versatility of soft robots to grip unclear objects, walk on uneven surfaces, or interact with humans. Further research on mathematical models of these continuously deformable robots is ongoing to predict their performance in real life and operational situations. In particular, the models should be able to describe nonlinear material properties, contact situations and the dynamic behavior of the soft robot in action, which is a major challenge.

At the Institute of Applied Structural Mechanics soft robots are investigated numerically and experimentally. In order to investigate the locomotion and interactions between the soft robot and its environment, a pneumatically actuated quadruped soft robot was manufactured and analyzed. In addition, its deformation and locomotion is described by Euler's rod model. Due to the simplified representation of the structure of the soft robot, some model parameters, such as the pressure-induced intrinsic curvature and the bending stiffness, have to be identified experimentally.

In addition, Majidi et al. have shown the significant influence of the friction coefficient on the locomotion of a quadruped soft robot. Depending on the friction behavior, their soft robot moves forwards, backwards or remains at the same position by the same actuation [1].

Therefore, in this paper, basic measurements of the friction behavior of the fabricated quadruped soft robot are performed in different actuation phases. In order to analyze the dependence on the momentary actuation, the coefficient of friction is related to the deformation of the robot which shows a nonlinear characteristic. The results are used in Euler's Elastica model to describe the contact between the soft robot and the surface more precisely. In addition, investigations on the locomotion of the soft robot with different friction behavior are carried out numerically. The experimental investigations are particularly important to describe the quasi-static and dynamic behavior of the soft robot during locomotion.

[1] C. Majidi. The International Journal of Robotics Research, 32, 13, 1577-1584 (2013).

Vibrational influence on the friction forces during disk brake squeal

Thai Minh Tuan Nguyen (*Technische Universität Berlin, Germany*)

16:50

Nils Gräßner (*Technische Universität Berlin, Germany*)

Utz von Wagner (*Technische Universität Berlin, Germany*)

During brake squeal, in addition to the motion between the rotating brake disk and the fixed brake pads, vibrations of both parts appear in various directions including the tangential direction. Since brake squeal is considered as the result of friction-induced vibration, in order to study the nature of this phenomenon, it is important to investigate the effects of vibration on the friction forces.

A corresponding test rig, called Oscillating Friction Test Rig (OFTR) was built up at the chair of Mechatronics and Machine Dynamics (MMD) that replicates this behavior. In this test rig, special focus is given on tangential vibrations of the pad excited by a piezoceramic actuator. With this OFTR, two effects were found, namely friction reduction and tangential friction-induced damping. These phenomena cannot be explained with known simple models of friction, making it hard to simulate the impact of these phenomena on brake squeal so that a special approach was proposed for calculation. Simulations were performed for multiple body models of a brake system. The results show that, in case of brake squeal, these nonlinearities may restrict the vibration of the brake system to a limit cycle.

Bifurcations and limit cycles due to self-excitation in nonlinear systems with joint friction: initialization of isolated solution branches via homotopy methods

Jonas Kappauf (*University of Kassel, Germany*)

17:10

Hartmut Hetzler (*University of Kassel, Germany*)

Considering nonlinear dynamical systems, a steady state solution can become unstable, e.g. by crossing a Hopf-bifurcation point. Then, the nonlinearities restrict the growth of amplitude and can cause periodic limit cycles due to a particular self-excitation mechanism. Usually, dynamical systems in engineering applications exhibit a certain amount of dissipation caused by material or frictional damping. Here, dry friction in joints and contacts is considered and understanding its influence on the bifurcation behaviour of stationary solutions is addressed.

For the approximation of periodic limit cycles, suitable methods, e.g. averaging or harmonic balance methods (HBM) exist and can be applied for various types of nonlinearities, especially non-smooth forces. When considering non-smooth friction, isolated solution branches can occur, and it is hard to find sufficient initial conditions to initialize continuation of such branches. In the residual equations of the HBM, friction can be treated as a perturbation of the underlying smooth problem. Hence, homotopy methods are applied, which allow a unique transition map from a known solution of the smooth problem to the isolated solution branch.

Within this contribution, the HBM is applied to low degree of freedom systems showing self-excited periodic limit cycles under the influence of non-smooth joint friction. In terms of evaluating the Fourier coefficients of the nonlinear forces for HBM the Alternating-Frequency/Time scheme is applied and a classical predictor-corrector continuation is used for calculating a certain solution path. Moreover, the bifurcation behaviour is analysed. To this end, the detection of isolated solution branches via homotopy is presented for several low degree of freedom systems and an outlook to analysis of large scaled systems is given.

Modeling of the stick-slip motion of an oscillatory roller during soil compaction

Ivan Paulmichl (*University of Innsbruck, Austria*)

17:30

Christoph Adam (*University of Innsbruck, Austria*)

Dietmar Adam (*TU Wien, Austria*)

A roller, also referred to as roller-compactor, is a heavy equipment used for near-surface compaction of soil layers in the construction of roads, airfields, dams, track foundations, etc. In this contribution, a lumped parameter model of the interacting oscillatory roller-soil system is presented that captures the stick-slip motion of the drum during near-surface compaction of non-cohesive soils. In this model, the subsystem roller is represented by the oscillating drum and its viscoelastic connection to the roller frame. The deformed soil below the drum is predefined as a rigid curved track, supported by a vertical and a horizontal Kelvin-Voigt element. As such, also the vertical drum accelerations observed in the field can be simulated. Coulomb's law of dry friction is used to describe the contact between drum and soil surface. The numerical solution of the resulting three degrees-of-freedom lumped parameter model is found by switching between the sets of highly nonlinear ODEs for the stick and for the slip phase. Selected numerical results show the influence of the soil stiffness on the acceleration response of the oscillating drum with respect to compaction control techniques for oscillatory rollers.

On a simple nonlinear system with circulatory forces

Ahmed A. Barakat (*Technische Universität Darmstadt, Germany*)

17:50

Peter Hagedorn (*Technische Universität Darmstadt, Germany*)

Self-excited vibrations in mechanical system have been always gathering attention since being problematic for various applications, including brake squeal, aerodynamic flutter, machining chatter, and galloping transmission lines, or in some cases beneficial as in some musical instruments (ex. violin) or resonant MEMS. These vibrations can have different origins, such as 'negative damping' (such as in the classical Van der Pol oscillator) and/or circulatory forces (i.e. 'follower forces', non-conservative positional forces). Both the negative damping and the circulatory forces can have different physical origins. It is well known that frictional forces generated between bodies in sliding contact can generate circulatory terms as well as damping and other types of forces. In particular, if one of two bodies in frictional contact moves with a constant speed or angular velocity, the other one being capable to oscillate, this implies an energy source for the oscillating part of the system. This has been identified as the cause for many self-excited vibrations.

In this presentation a very simple nonlinear two-degree-of-freedom system of this general type is examined in some detail. It has recently been proposed in the literature as a paradigm for frictionally generated circulatory forces, for which the equations of motion can be derived from first principles. Other related systems have been presented in the literature before, but this newer system seems to be much simpler than the earlier ones and presents a great wealth of dynamic behavior. The nonlinear equations of motion of this 2dof system always have the trivial solution and, depending on the system's parameters, also non-trivial stationary solutions.

The stability of the different stationary solutions is discussed in some detail, and the non-linear system is also studied via different perturbational approaches (multiple scales and normal forms). It was interesting to note that the increase of the friction parameter drives the system towards instability. This does however not happen, if the stiffness of both springs are identical, which practically can't be guaranteed. Thus, a perfectly symmetrical system (with identical springs) is on the edge of instability, if the friction forces are large enough. Moreover, If the normal force responsible for the friction is not constant, but pulsating, with a time-constant and a harmonic component, an interesting parametrically excited nonlinear system is obtained.

Numerical simulation of vibro-impact problems using a massless boundary approach

Johann Gross (*University of Stuttgart, Germany*)

18:10

Carlo Monjaraz Tec (*University of Stuttgart, Germany*)

Malte Krack (*University of Stuttgart, Germany*)

The vibration simulation of flexible structures subjected to dry friction, unilateral contacts and impacts is a challenging task. Spatial discretization with conventional finite elements associates a finite mass to the nodes at the contact interface (mass-carrying boundary). Contact interactions then result in finite impulses which cause high-frequency oscillations. These oscillations, to a large extent, do not occur in the continuum case and are thus artificial. These artificial oscillations sabotage the accuracy and necessitate very small time steps during numerical integration.

One way to overcome this problem is to use structural models with a massless boundary. We propose using an appropriate component mode synthesis method which yields a massless boundary and permits a considerable model order reduction.

We use a Moreau-type time stepping scheme, which permits to directly take into account the set-valued contact laws without the need for regularization. First, we demonstrate the accuracy of the method for a one-dimensional bar with unilateral contact, for which the exact solution of the spatially continuous problem is known.

Then, we consider a three-dimensional beam with unilateral normal contact (Signorini law) and dry friction in the tangential plane (Coulomb law). We compare the results and analyze the computational effort of our method with time stepping applied directly to the initial finite element model or a conventional reduced order model (mass-carrying boundary).

S05.03 | Nonlinear oscillations

Date: February 20, 2019

08:30-09:30

Room: HS 16

Invariant manifolds in control problems

Alois Steindl (*TU Wien, Austria*)

08:30

Invariant manifolds are useful tools for the investigation of nearly all nonlinear systems. Especially for the determination of stabilizing controls the center-stable manifold characterizes the proper feedback controls.

The method is demonstrated for the stabilization of a tethered satellite in the local vertical position by applying tension control. While in-plane perturbations can be extinguished in finite time, the tension control acts as parametric excitation for out-of-plane perturbations and is only able to cause a slow algebraic decay for both kinds of perturbations. An analytical or numerical power series expansion of the center-stable manifold at the target state provides the proper feedback controls.

Nonlinear stability analysis of an oversteer automobile

Johannes Edelmann (*TU Wien, Austria*)

09:10

Alois Steindl (*TU Wien, Austria*)

Manfred Plöchl (*TU Wien, Austria*)

Giampiero Mastinu (*Politecnico di Milano, Italy*)

The steady-state motion of automobiles showing oversteer handling characteristics turns to be unstable at high lateral accelerations. To investigate the handling behaviour in this study, the basic two-wheel vehicle model including wheel dynamics and the tyre brush model is applied. Thus, the generalised motion variables are the longitudinal and lateral velocity, the yaw rate and the angular wheel speed. From including the longitudinal dynamics into the modelling, a supercritical Hopf bifurcation is found for a given oversteer vehicle for varied steering wheel input. At the minisymposium, the relation between the respective limit cycles and the unstable steady-state powerslide driving condition will be addressed as well.

S05.04 | Nonlinear oscillations

Date: February 20, 2019

14:00-16:00

Room: HS 16

Studies of lubricant flow and friction in partially filled gaps

Lukas Stahl (*Technical University of Brunswick, Germany*)

14:00

Michael Müller (*Technical University of Brunswick, Germany*)

Georg-Peter Ostermeyer (*Technical University of Brunswick, Germany*)

Starved lubrication is a friction regime in which the gap between the contact partners is not fully filled with fluid. Starved lubrication is an important strategy for minimizing the amount of lubricant needed, and also inevitably occurs during idling and fail-safe lubrication. In this regime, however, the flow of the lubricant and the related friction coefficients are yet to be fully understood. Strong non-linear behavior, transient influences and periodic effects occur and hamper the creation of a comprehensive theory. This presentation aims to make a fundamental contribution to the understanding of contact mechanics of partially lubricated contacts.

With two experimental setups on differing scales, the lubricant flow, the coefficient of friction (COF), and other variables were studied over a wide range of parameters. Distinct friction behaviors were observed on both scales, for example the typical characteristic of the Stribeck curve. The Stribeck curve shows the (COF) over the relative velocity and typically has a minimum of the COF at the mixed friction regime. In addition to this well documented behavior the experiments exhibits a similar phenomenon regarding the lubricant filling level in the gap. This leads to the conclusion that the friction regime can also be controlled by the fluid amount in the gap. To investigate this behavior the fluid was evaluated with still images from the experiments. This study exhibits distinct flow patterns for different friction regimes of starved lubrication.

Additionally, a model that evaluates the friction regime on both scales is presented. This model assesses the scalability of the studied friction problems. With this model phenomenological similarities between the flow patterns of the experiments and the simulations were found.

Comparison of dry friction models for the computational analysis of refrigerant-lubricated GFB rotor systems

Tim Leister (*Karlsruhe Institute of Technology (KIT), Germany, INSA Lyon, France*)

14:20

Wolfgang Seemann (*Karlsruhe Institute of Technology (KIT), Germany*)

Benyebka Bou-Said (*INSA Lyon, France*)

In response to growing industrial efforts of developing energy-efficient and oil-free turbomachinery, research on self-acting gas foil bearings (GFBs) has become a topic of great scientific interest. GFBs offer the benefit of almost wear-free operation with remarkably small damping, which is due to the fact that the high-speed rotor is borne by a thin lubricant film often consisting of gaseous refrigerants or similar low-viscosity fluids. On the other hand, the absence of any

major source of energy dissipation makes the strongly nonlinear rotordynamic system prone to instability scenarios resulting in self-excited subsynchronous vibrations. Acting as a kind of passive vibration control mechanism, the compliant and slightly movable foil structure inside the lubrication gap possesses an excitation-dependent ability of dissipating some of the excessive energy by means of deliberately introduced dry friction. In view of the resulting fluid–structure–rotor interaction problem, the computational analysis of rotating machinery using GFBs reveals to be a challenging task demanding fully monolithic simulation approaches. To this effect, the entire dynamical system must be described using one single autonomous first-order ordinary differential equation system, which is derived from three fully coupled fluid–structure–rotor submodels. Surprisingly, despite friction within the foil structure being of such crucial importance, almost none of the computational GFB models found in literature are capable of really capturing the switching nature of stick–slip transitions and hence suffer from inaccuracies when assessing the dissipated energy. The implementation of an elasto-plastic bristle friction law, recently proposed by the authors, provides indeed better quantitative results but is suspect to be unreasonably complex for the identification of qualitative effects concerning the overall system dynamics. This contribution addresses the arising conflict of simulation goals by incorporating multiple friction models with or without true stiction into the structural model, which is hereafter coupled to a Reynolds equation for non-ideal compressible gases and to a modified Jeffcott–Laval rotor. Conducting a systematic investigation making use of numerical bifurcation and stability analysis combined with solution continuation techniques and numerical time integration, comparisons and recommendations of appropriate friction models for different use cases are given. From a more general point of view, this study gives interesting and novel insights into the stationary and dynamic performance of modern refrigerant-lubricated GFB rotor systems.

Numerical analysis of vibration patterns in hydropower units

Christian Sperber (<i>Voith Hydro Holding GmbH & Co. KG, Germany, University of Stuttgart, Germany</i>)	14:40
Wilhelm Weber (<i>Voith Hydro Holding GmbH & Co. KG, Germany</i>)	
Peter Eberhard (<i>University of Stuttgart, Germany</i>)	

Every manufactured rotor shows some degree of unbalance and other imperfections that cause vibrations. In this contribution, a dynamic model is used to calculate the lateral vibrations of vertical rotors in hydropower units due to such imperfections. This is done to analyze how distinct shape deviations like unbalance and misalignment contribute to the overall vibration response.

One crucial aspect of such models are the hydrodynamic bearings, which show nonlinear behavior. In horizontal machines, the gravitational force will determine the steady position of the shaft within the bearings. Stiffness and damping coefficients of the bearing oil film can be linearized for that position. Linearization is not suitable for vertical rotors, like those in large hydro generators, since there is no constant radial static load. Instead, the radial load is highly dependent on hydraulic forces that change with the operating mode the power plant is currently running in. Non-linear hydrodynamic forces in the bearings are properly described by the Reynolds equation. However, its solution is expensive in terms of computing time. More efficient ways to handle the non-linear behavior of bearings in rotordynamic models are still under discussion in current research. They include linear or non-linear approximations of the forces obtained by the Reynolds equation or pre-calculated databases for those forces.

Further components to be modeled are the rotor shaft, the generator with acting electro-magnetic forces and the turbine. Also, imperfections like unbalance need to be considered in an appropriate way.

Using an adequate model, common shape deviations like unbalance and coupling misalignment are investigated and their corresponding rotor response is presented and discussed. The results

will be used for further research concerning fault identification in measured vibration data of hydro-electric machines.

Investigation of a centrifugal exciter with two coaxial unbalances on a carrier performing planar motion

Tunc Yüzbasioglu (*Karlsruhe Institute of Technology (KIT), Germany*)

15:00

Olga Drozdetskaya (*Karlsruhe Institute of Technology (KIT), Germany*)

Alexander Fidlin (*Karlsruhe Institute of Technology (KIT), Germany*)

The passing through and capturing into the resonance of rotating machines is an important topic for scientific research, which is also relevant for industrial use. To avoid the capture into resonance, known as Sommerfeld effect, which may prevent the system to reach the operating point, the dynamics of such systems should be examined thoroughly.

The current work is the continuation of [1], which investigated a minimal model of a centrifugal exciter. The model in this paper consists of an unbalanced rotor, driven by an induction engine of limited power, with an additional pendulum unbalance mounted on it. The rotor is installed on a strongly damped oscillatory carrier, which can perform planar motion.

The dynamics of the system is investigated using an averaging method for partially strong damped systems. The system exhibits additional stationary and periodic solutions in vicinity of the resonances of the carrier system, which isn't found in the system with one degree of freedom of the carrier system, see [1]. The objective is to analyze these additional solutions and their existence domain subject to system parameters by investigating the phase space.

[1] Drozdetskaya, O. and Fidlin, A., 2018. On the passing through of a centrifugal exciter with two coaxial unbalances. *European Journal of Mechanics / A Solids*, 72, 516 - 520

Oscillations in a system of two coupled self-regulating pressure control valves with switching behaviour

Simon Schröders (*Karlsruhe Institute of Technology (KIT), Germany*)

15:20

Alexander Fidlin (*Karlsruhe Institute of Technology (KIT), Germany*)

In hydraulic systems valves can be considered as fundamental components. They serve as control elements to regulate hydraulic power transmission. To minimize control effort, self-regulating valves enjoy great popularity. Their disadvantage is a possible loss of stability induced by the coupling between hydraulic and mechanical degrees of freedom via pressure feedback areas. This leads to the occurrence of self-excited vibrations at certain operating points or in case of unfavourable parameterization.

So far, this problem has mostly been investigated using minimal models of individual valves. Critical parameters which influence the stability could be identified there. However, since parameters can change during operation, stable operation cannot always be assured.

In real world applications, for example in automotive transmissions, typically several valves with pressure feedback areas are employed which are coupled to each other by the hydraulic pipes connecting them.

This contribution discusses a model consisting of two coupled self-regulating valves. The valves are modelled as ideal in the sense of leakage characteristics, resulting in a non-smooth mathematical model describing them. Both valves can separately perform self-excited oscillations for certain parameter configurations.

The aim of this study is to investigate the influence of different parameters, such as the coupling strength between the two oscillators, on the stability and the dynamic behaviour of the overall system.

It is shown that with weak coupling between the two valves oscillations are synchronized, whereas with stronger coupling complex and possibly chaotic oscillations can occur.

A geometrical nonlinear model for rotating cylindrical shells

Rico Schmidt (*TU Bergakademie Freiberg, Germany*)

15:40

Alfons Ams (*TU Bergakademie Freiberg, Germany*)

Shell structures are extensively used in engineering for constructions with light weight and high strength. Classical applications are covers in automotive industry, aero- and astronautics. For this purpose the dynamical behavior is of interest for safety and comfort. The focus will be placed on rotating circumferential cylindrical shells.

Starting with the geometrical nonlinear kinematics for the strains, the Hamilton's principle is evaluated. In the following-up to the calculus of variations Ritz approach is used, to compute eigenfrequencies. Afterwards the results are discussed for certain examples and compared to FE-solutions.

S05.05 | Nonlinear oscillations

Date: February 20, 2019

16:30-18:30

Room: HS 16

Aeroelastic limit-cycle oscillations of piezoelectric energy harvesters

Andreas Zilian (*University of Luxembourg, Luxembourg*)

16:30

A specific class of energy harvester devices allows conversion of fluid flow energy to electrical energy by utilising flow-induced vibrations of a piezo-ceramic structure positioned in the flow field. This energy converter technology simultaneously involves the interaction of a composite structure and a surrounding fluid, the electric charge accumulated in the piezo-ceramic material and an electrical circuit that represents the attached electric consumer/storage/controller backend. This contribution discusses a monolithic model for simultaneous analysis of nonlinear oscillations of thin-walled harvesters subject to surface-coupled fluid and structural dynamics, volume-coupled electro-mechanics and a controlling energy harvesting circuit. The aeroelastic problem is described using a finite state aerodynamic theory for incompressible, two-dimensional flow around a thin-walled object for which the resulting set of first-order state equations is coupled via the deformation-dependent pressure distribution to an elastic Euler-Bernoulli beam with piezoelectric layers attached in uni- or bimorph configuration. The electric potential collected on the electrodes, covering the piezoelectric patches, is coupled to a simplified electric circuit, represented by a resistor element. Accounting for moderately large deformations the resulting model exhibits nonlinear structural stiffness together with nonlinear added aerodynamic damping and mass.

The overall model is employed to study the response characteristic of the coupled harvester system in the vicinity of critical flow velocities, indicating the onset of flutter and predicted by linear stability analysis. Investigation of associated limit-cycle states allows to estimate magnitude and sensitivity of the achievable electric power output under a broader spectrum of flow velocities.

A time-integration algorithm for non-linear dynamic systems of first and second order

Helmut J. Holl (*Johannes Kepler University, Austria*)

16:50

Non-linear dynamic systems are defined by mechanical models involving differential equations of second order and also first order differential equations are present frequently. Such systems are derived when some degrees of freedom have a corresponding small mass or even no mass. Also if the stiffness parameter is not present in the equations or if a controller is implemented in the system differential equations of first order are present. Some applications are in biomechanics and in connection of dynamic mechanical systems with biological and chemical processes. For linear systems of first and second order a variety of solutions is presented in [1].

A semi-analytical method is presented which is exact for the linear dynamic systems described by coupled differential equations of first and second order. A modal transformation of the equations is necessary after a suitable partitioning of the system equations. After a discretisation in the time-domain the relevant equations for a suitable and effective time-integration algorithm are defined which considers the non-linearity. The resulting procedure is derived and the used formulation is analogous to the BEM-formulation in time, described in [2] for a system of second order only. In this contribution the method is extended to the coupled non-linear differential equations of first order. Analogous to the analysis of the semi-analytic time-integration method for variable mass non-symmetric and non-linear systems in [3] the present method is analysed with respect to the numerical behaviour. In contrast to other known time-integrations methods this algorithm is exact for linear systems. The analysis of the numerical behaviour of the algorithm is analysed for a defined non-linearity and additionally the stability and accuracy of the algorithm is demonstrated. The resulting algorithm is applied to a representative example and some solutions are compared with well-known numerical methods.

References:

- [1] Angeles, J., Dynamic Response of Linear Mechanical Systems. Modeling, Analysis and Simulation, Springer, 2011.
- [2] Holl, Helmut J.; Belyaev, Alexander K.; Irschik, Hans: Simulation of the Duffing-Oscillator with Time-varying Mass By a BEM in Time. Computers and Structures 73, 177-186, 1999.
- [3] Holl, Helmut J., Analysis of Variable Mass Rotordynamic Systems with Semi-Analytic Time-Integration. Proceedings of the 10th International Conference on Rotor Dynamics - IFToMM, eds. Cavalca K.L., Ingo Weber, H. I., Vol. 3, 412-425, 2018.

Bouc hysteresis without an elastic restoring force under white noise excitation using the beta distribution

Christian H. Kasess (*Austrian Academy of Sciences, Austria*)

17:10

Holger Waubke (*Austrian Academy of Sciences, Austria*)

Elastic elements for decoupling of vibrating devices often show hysteretic behavior. This hysteretic behavior can be taken into account using the Bouc model where an internal elasto-plastic force is added to the equation of motion resulting in a system of three partially non-linear first-order differential equations for the displacement, the velocity, and the force-proportional displacement which describes the hysteretic force. With a suitable description of the force-displacement relationship hysteretic behavior is achieved.

Under white noise excitation the evolution of the probability density of the state variables can be derived comprising a set of coupled first-order differential equations for the statistical moments of this probability density. In order to use these equations, certain restrictions on the distribution have to be applied. The most straightforward, the Gaussian closure, approximates the density by a multivariate Gaussian and thus higher order moments are given by the first two statistical moments. This allows for all necessary integrals to be solved analytically making it extremely efficient.

Although, the Gaussian Closure leads to good results, in the softening regime the force-proportional displacement is restricted to an interval and thus for large excitation levels the Gaussian distribution is not a suitable assumption for this variable. Alternatively, a moment

closure approach based on the beta distribution for the force-proportional displacement and a non-linear mapping from the force-proportional displacement to the displacement and the velocity can be defined. Similarly, the resulting distribution is defined by the moments up to order two. The main disadvantage is that four 1D integrals have to be calculated using a numerical quadrature resulting in a decreased efficiency.

This closure was shown previously to lead to good agreement with Monte-Carlo results in the case where an elastic restoring force is present. In the current work, the beta closure is applied to the case without an elastic restoring force, i.e. no stationary case exists. Results for different noise strengths and pre-stress values show good agreement for most of the statistical moments up to fourth order. However, there are significant deviations in some higher order central moments of the displacement and the velocity. The bivariate marginalized distributions show a close resemblance to the Monte-Carlo distributions which is in contrast to the Gaussian Closure where the main focus are the statistical moments.

Dynamical characteristics of electromechanical energy dissipation due to translatory motion: a minimal example

Felix Boy (*University of Kassel, Germany*)

17:30

Hartmut Hetzler (*University of Kassel, Germany*)

Arnold Tchomgue Simeu (*University of Kassel, Germany*)

Electromechanical systems cover a broad technological range of application. Typical examples are electrical machines, electromagnetic shakers and dampers, eddy current brakes, or different types of actors and sensors. Their dynamical behaviour is affected by some very challenging peculiarities. Among these are inherent geometrical and physical non-linearities, as well as strongly differing timescales. Consequently, all these effects may result in different kinds of vibration issues.

Within this contribution, the classical textbook example of a magnetic circuit is combined with a simple mass oscillator to establish a minimal model for the type of systems discussed above. In this scenario, the translatory motion of the mass affects the air gap length of the circuit and in return, a magnetic force is exerted on the mass. Stationary solutions of this electromechanical system are calculated using the harmonic balance method and parameter variations are carried out. Furthermore the effect of magnetic saturation is taken into account.

The study shows many typical effects, which can also be observed in more complex systems as for example in electric machines. From this point of view, the minimal model may help to explain the underlying physical principles on a fundamental basis.

Steady state dynamics of pre-stressed, piezoelectrically excited circular plates - a harmonic balance approach

Florian Toth (*TU Wien, Austria*)

17:50

Manfred Kaltenbacher (*TU Wien, Austria*)

The investigated system consists of a circular plate-like structure with a diameter of several hundred micro meters with possible applications as a MEMS speaker. It is composed of several layers of different materials, typically a substrate, electrodes, and an active piezoelectric layer to apply dynamic loads. Using classical plate theory based on the Föppl-von Karman assumption for large displacements and taking into account Voigt's linearised piezoelectric constitutive relations, we obtain a geometrically non-linear plate theory. For circular symmetric plates, this can be reduced to a non-linearly coupled PDE system 2nd order in time, 4th order in the transverse displacement and 3rd order in radial direction.

The static equilibrium can be numerically solved using a collocation based boundary value solver, which allows to predict the buckling loads for static pre-stress, e.g. thermal stresses arising during

the production process. After a brief discussion of the encountered snap-through behavior, we aim to study the dynamics of the systems when oscillating close to a critical point.

We adopt a multi-harmonic ansatz and perform harmonic balancing to transform the PDE systems into a boundary value problem in space. This problem can be written as a first order system with 7 complex valued unknowns per considered harmonic. We employ above boundary value solver to obtain the steady state oscillation behavior for each base-frequency, and study it for a range of forcing frequencies. Additionally, we investigate the amplitude-dependent natural frequencies and mode shapes.

Experimental nonlinear modal analysis of structures with nonlinear dissipation

Maren Scheel (*University of Stuttgart, Germany*)

18:10

Malte Krack (*University of Stuttgart, Germany*)

In the light of material efficiency and light-weight structures, nonlinear vibration phenomena occur in, for example, slender or jointed structures and can no longer be neglected. To ensure safe operation, these nonlinearities must be considered when predicting vibrations. Measurements are indispensable to verify these predictions and identify parameters of nonlinear models. This can be achieved by one of the numerous methods for nonlinear system identification. One approach is nonlinear modal analysis.

The concept of nonlinear modes can be used to determine natural frequencies, damping ratios and modal deflection shapes as function of the vibration level, and to understand and characterize certain nonlinear vibration phenomena (Kerschen et al., *Mech Syst Signal Process*, 2009). Different definitions for nonlinear modes exist. Most commonly, a nonlinear (normal) mode is defined as periodic motion of an autonomous system. Since real-life structures are always damped, the autonomous motion will decay and no longer be periodic. Therefore, an extension of the periodic motion concept had been proposed (Krack, *Comput Struct*, 2015): The motion of a damped autonomous system is made periodic by introducing an appropriated negative damping to the system, compensating for all natural dissipative effects. This definition is consistent with the linear case under modal damping and it was shown that the modal properties accurately represent the vibration behavior close to an isolated resonance under external forcing or self-excitation. However, in case of high damping and, at the same time, modal interactions, this mode definition might not give meaningful results.

At the conference, we will present an experimental realization of the extended periodic motion concept where the negative damping term is interpreted as external force (Scheel et al., *J Sound Vib*, 2018). As an approximation, only a single-point, single-frequency force is applied to the system. The phase lag between force and response is controlled to drive the system into (phase) resonance. Once the controller is locked, the steady-state vibration is recorded, and modal properties are extracted from the measurements: The frequency and deflection shape are measured directly. The damping ratio is defined based on the dissipated power in the system which is equal to the measured excitation power. By applying the method to different test specimens, we show that the extracted modal properties are in fact meaningful to describe forced responses around isolated resonances. In the presentation, we will also address limitations of the current experimental approach.

S05.06 | Nonlinear oscillations

Date: February 21, 2019

08:30-10:30

Room: SR 06

Modeling and simulation of metal bellows in vacuum interrupters

Aydin Boyaci (*ABB AG, Germany*)

08:30

Christian Simonidis (*ABB AG, Germany*)

Dietmar Gentsch (*ABB AG, Germany*)

In vacuum interrupters, metal bellows permit the motion of the moving contact with long contact strokes while maintaining the ultra-high vacuum seal. In contrast to most other bellows applications, the opening and closing operation of the vacuum interrupter lead to high-impulsive motions which additionally excite bellows oscillations. Future requirements of longer strokes and higher velocities demand for a simulation-driven optimization of the metal bellows to increase the mechanical lifetime of the vacuum interrupter.

A mechanical FE model of the bellows is considered to investigate the damaging effect of the switching operations. In the validation step, a static force is axially applied on the one-sided fixed bellows to determine the axial stiffness compared with experimental results. Furthermore, a modal analysis is performed to provide a classification of bellows modes. To account for the multiple-frequency oscillations during the switching operation, a transient simulation is carried out where the excitation of the bellows follows from a travel curve. For this loading case, the hot spots of mechanical stresses are identified. Finally, parameter studies show a significant effect of wall thickness variation on the mechanical stresses.

Nonlinear thermomechanical vibrations of bimodular beams

Rudolf Heuer (*TU Wien, Austria*)

08:50

The present paper is concerned with the modelization and numerical solution of the transient response of Bernoulli-Euler beams due to thermal excitation. The beam is assumed to be homogeneous and simply supported. However, it is composed of a bimodular material, thus behaving differently in tension and compression. Assuming a time-variant (nonlinear) temperature distribution across the beam's cross-section its influence is considered by defining cross-sectional means of thermal strain and thermal curvature. When deriving the equations of motion for flexural oscillations an advanced procedure is developed by defining an effective composite layered structure with discontinuous natural beam axis depending on the sign of deflection's amplitude. The position of the natural axis follows from a nonlinear equation that is dependent on both the geometry of the cross-section and the elastic material properties. By means of a semi-analytical method, using a modified Galerkin-procedure to discretize spatially and the Newmark beta method for time wise discretization, parameter studies are performed for the load cases "imposed time-harmonic thermal curvature" and "thermal shock". The results are compared to those derived with alternative integration schemes.

Nonlinear responses of metastructures with bistable attachments

Yiwei Xia (*Georgia Institute of Technology, USA*)

09:10

Massimo Ruzzene (*Georgia Institute of Technology, USA*)

Alper Erturk (*Georgia Institute of Technology, USA*)

Grzegorz Litak (*Lublin University of Technology, Poland*)

The elastically coupled five mass structure with bistable magnetoelastic beam attachments is subjected to harmonic kinematic excitation. The system is simulated numerically. We show various solutions by using wavelets and relative phase synchronization. Depending on the excitation amplitude we observe various periodic and chaotic responses. Generally, the metastructure response follows a linear bandgap under low amplitudes and nonlinear attenuation by attachments under larger amplitude. In the second case various complex interactions are manifested, altering the attenuation performance.

S06 | Material modelling in solid mechanics

Organiser: Thomas Antretter (*Montanuniversität Leoben, Austria*)
Clara Schuecker (*Montanuniversität Leoben, Austria*)

S06.01 | Material modelling in solid mechanics

Date: February 19, 2019
Room: BIG HS

08:30-10:30

A thermomechanical modelling framework for selective laser melting based on phase transformations

Isabelle Guschke (*TU Dortmund University, Germany*) 08:30
Thorsten Bartel (*TU Dortmund University, Germany*)
Andreas Menzel (*TU Dortmund University, Germany, Lund University, Sweden*)

Additive manufacturing has a great potential for industrial applications, as the workpiece is directly manufactured layer by layer in contrast to traditional manufacturing techniques. Selective laser melting (SLM) represents one possible process to manufacture complex metallic parts, where the powder particles are selectively molten with a laser beam. The complexity of SLM arises from the interaction of several physical processes and in particular from the presence of high temperature gradients. Therefore, it is necessary to use an appropriate material model that captures the heat source and the transformations between the powder, molten and re-solidified phase, in particular a model that takes account of the significantly different mass densities of each phase.

In this contribution, the changes of the material states are regarded as solid-solid phase transformations adopted from approaches used for shape memory alloys, cf. [1]. Thus, the constitutive behaviour for each phase, namely powder, molten and re-solidified material, is modelled via phase energy densities. The overall constitutive model is based on a mixture rule/homogenisation approach. An averaged energy density is minimised with respect to the strains and phase fractions of each phase, see e.g. [2]. The minimisation problem with inequality constraints regarding to the range of the phase fraction and total strains is solved via the Karush-Kuhn-Tucker approach, which can be rewritten by the Fischer-Burmeister nonlinear complementarity functions.

With this approach at hand, the constitutive model is implemented into the commercial finite element software Abaqus. A fully coupled thermomechanical framework is used to capture the temperature evolution and eigenstresses in the additively manufactured part. In order to conduct SLM process simulations, various subroutines provided by Abaqus need to be used. This includes the definition of the specific material model, the application of the layer build-up as well as the modelling of the moving volume-distributed heat source. This model is capable of generating representative examples, where the evolution of temperature, eigenstresses and the explicit material state can be predicted.

[1] T. Bartel and K. Hackl. A micromechanical model for martensitic phase-transformations in shape-memory alloys based on energy-relaxation. *Journal of Applied Mathematics and Mechanics*, 89:792-809, 2009.

[2] T. Bartel, I. Guschke, and A. Menzel, Towards the simulation of Selective Laser Melting processes via phase transformation models. *Computers & Mathematics with Application*, available online, 2018.

A variational material model for shape memory alloys under thermal cycling

Johanna Waimann (*RWTH Aachen University, Germany*)

08:50

Klaus Hackl (*Ruhr-Universität Bochum, Germany*)

Philipp Junker (*Ruhr-Universität Bochum, Germany*)

Due to their special material behavior - namely the superelasticity as well as the one-way and two-way effect - shape memory alloys are very attractive materials for industrial applications. The solid/solid phase transformation between austenite and martensite is however accompanied by a formation of dislocations which influence the cyclic behavior of this special class of smart materials. For mechanical cycling, the formed dislocations favor the transformation from austenite to martensite and delay the reverse transformation. But for thermal cycling, they have the opposite effect and thus result in a decrease of the transformation temperature and in a delayed transformation from austenite to martensite.

We present a material model which is able to show both effects and hence display microstructural evolution for a mechanically and thermally cycled material. Based on the variational method of the principle of the minimum of the dissipation potential, we model the so called effect of functional fatigue by storage of the transformation history of the observed material. In addition to that and for numerical efficiency, we use an evolving orientation distribution function to account for the polycrystalline structure of shape memory alloys, see [1]. Our talk will be completed by the presentation of various numerical results which varifies the micromechanical model's functionality.

[1] P. Junker. A novel approach to representative orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys. *Int. J. Numer. Meth. Eng.* 98(11) (2014), 799-818.

Martensitic transformation at a crack under mode I and II loading

Simon David Schmidt (*TU Kaiserslautern, Germany*)

09:10

Wolfgang Dornisch (*TU Kaiserslautern, Germany*)

Ralf Müller (*TU Kaiserslautern, Germany*)

Metastable austenitic steels can undergo phase transformations. As an allotrope two crystal configurations are of interest: the softer austenitic parent phase and the martensitic phases. Here, the bain orientation relationship leads to distinct orientations for the martensitic variants with a different transformational strain. [1]

A phase field approach is used to model the transformation, where a multi-valued order parameter ϕ identifies the austenitic parent phase and the martensitic variants. This allows to define bulk and surface energies as regularized functions in terms of the order parameter and its gradient. The kinetics of the martensitic transformation are temperature dependent. Temperatures below an equilibrium temperature favor the growth of the martensitic phase, whereas temperatures above an equilibrium favor the austenitic phase. Approaching the equilibrium temperature slows the transformation down. [2]

In this work we consider a static crack under mode I and mode II loading for different temperatures. Numerical examples illustrate the behaviour of the martensitic transformation in the vicinity of the crack tip and surface. The field equations are solved using the finite element method. The model is implemented in FEAP as a 2D 4-node element with a bi-linear ansatz.

References

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[2] S. Schmidt, W. Dornisch, R. Müller [2017] "A phase field model for martensitic transformation coupled with the heat equation", *GAMM-Mitteilungen*, 40(2), 138-153

Modeling of electric field-induced magnetization switching in multiferroic heterostructures

Wolfgang Dornisch (*TU Kaiserslautern, Germany*)

09:30

Ralf Müller (*TU Kaiserslautern, Germany*)

Multiferroic heterostructures consist of materials with either pronounced ferroelectric or ferromagnetic effect. The combination of both types of material, be it in layers, columns or inclusions, potentially yields a significant magneto-electric coupling effect even at room temperature. The magnetization in the ferromagnetic material can be controlled by the application of electric fields to the ferroelectric material. In this contribution a linear elastic continuum formulation is coupled with a phase field formulation for the polarization and magnetization in the ferroelectric and the ferromagnetic layer, respectively. The strain transfer at the interface of the layers yields a magneto-electric coupling effect within the heterostructures. The finite element method is used to discretize the arising differential equations. Numerical examples show the peculiarity of the interpolation of the length-constrained magnetization vector and provide a proof of concept for the simulation of the magneto-electric coupling effect in multiferroic heterostructures.

Open problems in constitutive modelling of martensite

Manuel Petersmann (*Montanuniversitaet Leoben, Austria*)

09:50

Thomas Antretter (*Montanuniversitaet Leoben, Austria*)

Georges Cailletaud (*MINES ParisTech, France*)

Aleksandr Sannikov (*Montanuniversitaet Leoben, Austria*)

Many alloys exhibit a martensitic solid state transformation, which has crucial consequences on their mechanical behavior and is in further consequence of high technological importance in many applications. In some alloys, such as certain steels, the martensitic transformation is strongly coupled to plastic deformation, i.e. dislocation motion. Consequently a multi-mechanism treatment becomes necessary. A crucial, but hard to capture point is a proper coupling between the mechanisms of transformation and plasticity. Geometrical considerations on the lattice and the experimentally observed microstructure (on the micro and meso scale) are used to develop proper relations. To avoid an exploding computational cost on scaling up the problem, phenomenological relations are necessary at some point. However, they must be backed up by geometry resolving full-field models or experimental data. An example of a stress scaling relation for evolving martensite fraction is presented. The multi-scale and multi-mechanism nature of the problem leads to a highly ill-posed inverse parameter fitting procedure. Therefore, physical relations and reliable experimental data are crucial. However, experimental determination of microstructurally useful data for micromechanical martensite models is highly complex. The problem of indistinguishable martensite variants, out of the exploding available digital data of orientation imaging microscopy, is elaborated. The term crystallography-microstructure-relationship is introduced and emphasized in this regard. A future interplay between physics based deterministic models and machine-learning approaches is emphasized.

S06.02 | Material modelling in solid mechanics

Date: February 19, 2019

16:30-18:30

Room: BIG HS

Gradient enhanced crystal plasticity in additive manufacturing: identification of a macroscopic yield criterion

Andreas Kergaßner (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*) 16:30

Julia Mergheim (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

Paul Steinmann (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

Selective electron beam melting represents an additive manufacturing process and complex parts are built in a layer-wise manner using metal powders. The powder is fused selectively by the energy of an electron beam guided by electromagnetic fields. The so called electromagnetic lens allows for a very fast deflection and thus very high beam velocities and different scan strategies. By using these scan strategies it is possible to tailor the resulting mesostructure in the material which may range from a columnar to an equiaxed grain structure. For altered grain structures, different macroscopic mechanical properties are expected. Long grains oriented along the building direction cause highly anisotropic behavior. In contrast, a uniform grain structure results in isotropic mechanical behavior. Furthermore, different orientations of the unit cells, the effects of grain size and boundaries influence the macroscopic mechanical properties. The parameter identification for material models taking these effects into account is experimentally expensive. Thus isotropic material models are often used for process simulations, simulations of parts or topology optimizations. To overcome this limitation a validated mesoscopic model has been developed which is used to identify the parameters of a suitable material model.

The Finite Element Method together with grain structures from numerical grain growth simulations are used to simulate columnar grained IN 718, a face-centered-cubic nickel base alloy. On the mesoscale, the mechanical behavior is modeled using a gradient-enhanced crystal-plasticity model, allowing for relative misorientations on the grain boundaries. Computational homogenization and macroscopic experimental data are used to inversely identify elastic and plastic meso- and microscopic mechanical parameters. With this model at hand the macroscopic yield locus in the six dimensional stress space is identified as surface of constant dissipation and simulated for different values of dissipation. A multi surface yield function is fitted to the obtained results. A potential field of application is to extend standard topology optimization with information regarding preferred directions of the anisotropic material, which allows aligning these orientations based on the requirements on the parts.

A comparative study of integration algorithms for finite single crystal (visco-)plasticity

Stefan Prüger (*TU Bergakademie Freiberg, Germany*) 16:50

Björn Kiefer (*TU Bergakademie Freiberg, Germany*)

Developing robust stress-update algorithms for constitutive models at the single crystal scale, employing either rate-dependent or rate-independent formulations, is a particularly challenging task [1]. This is due to the fact that the inelastic deformation is governed by slip on a large number of distinct slip systems, each of them being controlled by an associated yield function.

However, if more than five slip systems are activated in case of isochoric inelastic deformation, the choice of active systems is no longer unique, resulting in the Taylor ambiguity problem, cf. [2]. The yield surfaces, that are essentially hyper-planes in stress space form corners at such points and the number of intersecting hyper-planes may exceed five. Moreover, incorporating anisotropic hardening into the constitutive model also significantly influences the evolution of the elastic domain,-making the choice of active slip systems even more complicated-, because of the complex interaction between different slip systems introduced by the hardening law.

In the current contribution different algorithmic treatments of a single crystal plasticity model are compared, employing an augmented Lagrangian formulation [3] and a formulation based on nonlinear complementary functions [4,5] in the rate-independent case, whereas in the rate-dependent case the formulations due to Perzyna [6] and Ortiz [7] are utilized. The influence of the anisotropy, both in terms of hardening law and elastic behavior, on the performance of the developed stress integration algorithms is assessed by means of representative numerical examples.

[1] Miehe, C., Schröder, J., “A Comparative Study of Stress Update Algorithms for Rate-Independent and Rate-Dependent Crystal Plasticity”, *Int J Numer Methods Eng*, 50(2), pp. 273-298, 2001

[2] Mánik, T., Holmedal, B., “Review of the Taylor Ambiguity and the Relationship between Rate-Independent and Rate-Dependent Full-Constraints Taylor Models”, *Int J Plast*, 55, pp. 152-181, 2014

[3] Schmidt-Baldassari, M., “Numerical Concepts for Rate-Independent Single Crystal Plasticity”, *Comput Methods in Appl Mech Eng*, 192(11), pp. 1261-1280, 2003

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[7] Cuitino, A. M., Ortiz, M. “Computational Modelling of Single Crystals”, *Model Simul Mater Sc*, 1(3), pp. 225-263, 1993

On the implementation of rate-independent gradient-enhanced crystal plasticity theory

Volker Fohrmeister (*TU Dortmund University, Germany*)

17:10

Jörn Mosler (*TU Dortmund University, Germany*)

For multiple reasons, e.g. for regularizing pathological mesh-dependencies in the case of material softening or for deriving dislocation densities based hardening models, there exists an increased interest in the incorporation of a certain length-scale into standard local crystal plasticity material models. This can be implemented, e.g., by taking into account the gradients of the plastic slip. While a naïve and straightforward implementation of these gradients would result in inequalities at the finite element level (due to rate-independent plasticity theory), a penalty formulation is presented which leaves the structure of the underlying local plasticity model unaffected, i.e., the respective inequalities are restricted to the material point level, see [3]. By doing so, the implementation of the gradient-enhanced model is almost identical to that of the original local one. For this reason, problems due to the determination of the active slip systems are not eliminated but inherited, cf. [1]. In order to solve such problems - and in line with [2] - the inequalities are transformed into an equivalent nonlinear complementarity problem.

[1] J. Schröder and C. Miehe, Aspects of computational rate-independent crystal plasticity, *Computational Materials Science*, Vol. 9, pp. 168-176, 1997.

- [2] M. Schmidt-Baldassari, Numerical concepts for rate-independent single crystal plasticity. *Computer Methods in Applied Mechanics and Engineering*, Vol. 192, pp. 1261-1280, 2003.
- [3] O. Aslan, N.M. Cordero, A. Gaubert and S. Forest, Micromorphic approach to single crystal plasticity and damage, *International Journal of Engineering Science*, Vol. 49, pp. 1311-1325, 2011

Multi-level thermomechanical material modeling to study heterogeneous plastic deformation of DP600 steel and effects of residual stresses on its mechanical properties

Shahbaz Ahmed (*TU Dresden, Germany*)

17:30

Stefan Löhnert (*TU Dresden, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

To determine the residual stress state resulting from incompatible plastic deformation in dual phase steel DP600, a simulation of the polycrystalline microstructure is carried out by applying cyclic loading. A macroscopic thermo-mechanically coupled material model is utilized which is motivated by a microscopic crystal plasticity model. Therefore, plastic deformation is taken into account for mixed isotropic and kinematic aspects in both, the macro and the microscopic model. A hysteresis of the effective mechanical response is calculated using an isothermally deforming RVE which consists of Voronoi cells as an artificially generated microstructure. A large difference of plastic flow between martensite and ferrite is observed which describes heterogeneity between these dissimilar phases. For detailed observation, the locally acting stress states which are composed of residual stresses are evaluated. In the end, a possibility of future extension of the macroscopic material model motivated by microscopic characteristics is investigated.

Test-based development in material modeling

Lukas Friedrich David Munk (*Leibniz Universität Hannover, Germany*)

17:50

Darcy Beurle (*Leibniz Universität Hannover, Germany*)

Silvia Reschka (*Leibniz Universität Hannover, Germany*)

Stefan Löhnert (*Technische Universität Dresden, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

FE simulations of highly complex material structures involve substantial programming efforts in sophisticated frameworks. Numerical software written by mechanical engineers is often not designed for robustness but rather for maximal scientific progress in the short-term.

A full simulation usually requires a long tool-chain of pre- and main-processing. Modifications to parts of the code in one location leads to unforeseeable errors in other modules or subroutines. Legacy code from former projects is often the most difficult to reuse, if at all, since working simulation cases are missing. In the worst case, scientific programmers have to understand from the source code how it is meant to be treated which is not always straightforward.

Aiming at a two-scale model of a nickel-based superalloy based on the eXtended Finite Element method and crystal plasticity, a partly automated testing environment will be presented. All consistent tangents are automatically generated in AceGEN and linked to FEAP. A range of possibilities on how to test FE simulations will be shown which are a step forward to cope with complexities in material modeling. This is common practice in large FE frameworks like deal ii.

Small strain crystal plasticity based on the primal dual interior point method

Lisa Scheunemann (*Universität Duisburg-Essen, Germany*)

18:10

Paulo S.B. Nigro (*Universität Duisburg-Essen, Germany*)

Jörg Schröder (*Universität Duisburg-Essen, Germany*)

Paulo M. Pimenta (*University of Sao Paulo, Brazil*)

Single crystal plasticity, which plays a major role in the analysis of material anisotropy and texture evolution, treats each crystalline grain, having a distinct orientation, individually. The polycrystalline material response is obtained upon considering a structure consisting of various individual grains, often also considering interface effects at the grain boundaries. On the individual grain level, single crystal plasticity can be treated in the mathematical framework of multisurface plasticity, leading to a constrained optimization problem wherein multiple constraints are defined as yield criteria on the different slip systems. Different approaches have been established in this field, see, e.g., [2], [3]. In rate-independent models, the set of active slip systems in the grain is possibly nonunique and is identified in, e.g., an active set search. Rate dependent approaches are based on power-type creep laws which do not differentiate into active or inactive slip systems. However, the constitutive equations of these formulations are often very stiff and require a small time increment. Here, a new algorithm for the solution of the constrained optimization problem based on the primal dual interior point method (PDIPM), [1], involving slack variables is presented for the framework of small strain single crystal plasticity. The use of slack variables therein stabilizes the conventional method and allows for a temporary violation of the constraint during the optimization. The optimization is solved using a Lagrange functional, wherein the nonlinear system of equations resulting from the derivation of the Lagrange functional is linearized using Taylor expansion and solved by a Newton Raphson scheme. All slip systems are considered simultaneously, omitting an iterative active set search. PDIPM has been found to lead to very efficient algorithms and better convergence rates than barrier or penalty methods. The stability of the algorithm would be especially beneficial in complex material models, such as a multiscale description of polycrystalline materials. Several numerical examples are presented showing the performance of the developed algorithm.

[1] El Bakry, A.S., Tapia, R.A., Tsuchiya, T. and Zhan, Y.: On the formulation and Theory of the Newton Interior Point Method for Nonlinear Programming. *Journal of Optimization Theory and Applications*, 89 (1996), 507-541.

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S06.03 | Material modelling in solid mechanics

Date: February 20, 2019

08:30-09:30

Room: BIG HS

An invariant-based formulation for transversely isotropic microsphere models with application to biomechanics

Christian Bleiler (*University of Stuttgart, Germany*)

08:30

Oliver Röhrle (*University of Stuttgart, Germany*)

Multiscale approaches for the modelling of materials like rubber or soft biological tissues often contain network models of continuously distributed chains or fibres on a small scale. Effective quantities, like the macroscopic strain-energy, are subsequently obtained by averaging operations over the surface of a unit sphere, thus justifying the common nomenclature *microsphere model*.

In this contribution, we present an invariant-based formulation for networks inheriting an equal fibre distribution in a plane orthogonal to a preferred axis under the affine deformation assumption. Thus, the model describes transversely isotropic materials and averaged macroscopic quantities may dependent on five scalar invariants.

After some theoretical considerations, the capabilities of the model for biomechanical applications will be shown.

Material model of pulp fibres

Tristan Seidlhofer (*TU Graz, Austria*)

08:50

Ulrich Hirn (*TU Graz, Austria*)

Manfred Ulz (*TU Graz, Austria*)

Paper is a natural product formed by a three dimensional network of fibres and shows a highly nonlinear and load-rate dependent behaviour. Neither the structure nor the fibre bonds can fully describe the time or rate dependent behaviour of paper [1]. Consequently, much experimental and numerical work was done to study the mechanics of a single fibre. As the fibre renders a viscoelastic, viscoplastic behaviour more advanced material models are necessary to evaluate material parameters.

Based on uniaxial tension tests [2] an appropriate one-dimensional plasticity framework is derived. The final model comprises a Perzyna type viscoplastic model with nonlinear hardening extended with a generalised Maxwell model to describe viscoelastic effects. The material properties are subjected to changes during plastic deformation. Hence, the model includes a damage/healing concept. The one-dimensional model shows a good performance and is ported to a finite strain three-dimensional formulation. We employ the framework of Hencky strains and a dual stress measure to ensure objectivity [3]. Finally, the model parameters are recalibrated with the one dimensional model. The investigation shows that pulp fibres have a distinct plastic behaviour, which could be the cause of the nonlinear behaviour on the macroscopic level of the network.

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[2] Dumbleton, D. F. (1972). Longitudinal Compression of Individual Pulp Fibres. Tappi, 55(1), 127-135.

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Thermo-mechanical modeling of pre-consolidated fiber-reinforced plastics for the simulation of thermoforming processes

Jean-Paul Ziegs (*TU Dresden, Germany*)

09:10

Daniel Weck (*TU Dresden, Germany*)

Maik Gude (*TU Dresden, Germany*)

Markus Kästner (*TU Dresden, Germany*)

Numerical optimization of the production process of hybrid lightweight structures consisting of metal and fiber-reinforced plastic (FRP) is of high importance. It can reduce the time to market and can also avoid the production of costly prototypes. To model the considered one-step thermoforming process, the deformation mechanisms of both components have to be determined. During forming of a plane textile-reinforced polymer into a three-dimensional shape, three basic deformation mechanisms - shear, tension and bending - can be observed. Since the material behavior of the polymer matrix is strongly temperature dependent, a high influence of the temperature on the deformation behavior is observed.

The material model employed to describe the behavior of the composite assumes an additive superposition of fiber and matrix contribution. The latter one is modeled by an elastic-plastic constitutive law with a Von-Mises yield criterion. The mechanical properties can be defined as temperature dependent. Fibers are described as an anisotropic non-linear elastic material with orientation vectors stored at the integration points. Their tension/compression and shear behavior are decoupled and can be defined by means of stress-strain curves and shear response as a function of shear angles of the fibers. Transverse shear moduli of the fibers can account for the typical low bending stiffness at temperatures above the melting point while still having a high in-plane tension stiffness.

Experimental data for the parametrization and validation of the modeling approach are the force-displacement curves under tensile loads as well as the shear force vs. shear angle curve. The characteristic behavior for in-plane tension is determined from tensile tests on strip specimens. The typically non-linear shear force vs. shear angle curves are recorded using the picture-frame test. Since the shear force of dry fabrics is mostly influenced by the contact of adjacent fibers, an additional shear resistance due to the polymer matrix can be observed for pre-impregnated composites. Gravimetric cantilever tests may be used to determine the temperature dependent bending stiffness.

The accordingly parameterized material model for the FRP is eventually applied in the simulation of thermoforming processes for the manufacturing of hybrid metal/FRP lightweight structures. The deformation behavior of the metal component is modeled by an anisotropic elastic-plastic constitutive law with a Hill48 yield criterion. Parameter studies show the influence of process parameters like forming temperature and binder force on the deformation behavior of the FRP and metal components and its tendency of the occurrence of defects like the formation of wrinkles.

S06.04 | Material modelling in solid mechanics

Date: February 20, 2019

14:00-16:00

Room: BIG HS

Numerical prediction of the homogenized orthotropic linear viscoelastic material properties of composite plies and laminated composites

Rainer Tomas (*Mück Kunststofftechnik GmbH, Austria*)

14:00

Melanie Todt (*TU Wien, Austria*)

Thomas Koch (*TU Wien, Austria*)

Heinz E. Pettermann (*TU Wien, Austria*)

Laminated composite components made of fiber reinforced plastics show a direction dependent creep and relaxation response as a consequence of the viscoelastic matrix material. Considering direction dependent viscoelasticity in finite element simulations on the component level requires a suitable constitutive law such as the one developed in [1]. This orthotropic linear thermo-viscoelastic material law is formulated under plane stress assumption making it especially suitable for shell based models mainly used in the simulation of composite structures.

The input to the constitutive model [1] in form of homogenized material data might be determined from experiments. However, the viscoelastic response of laminates depends not only on the material properties of the matrix and the fibers but also on the fiber volume fraction, the fiber orientation of the plies, and the layup. Consequently, the parameters have to be evaluated individually for each laminate making experimental procedures time consuming and inefficient. Herein, a homogenization procedure is proposed allowing to determine the required input parameters from a periodic unit cell approach reducing the experimental effort significantly. The only input data are the elastic properties of the fibers and the linear viscoelastic properties of the matrix. In a first homogenization step the effective plane stress properties of UD plies are computed using a generic periodic unit cell. With the so obtained material data the constitutive law [1] can readily be used together with layered shell elements to model composite components. Alternatively, the layered shell model can be utilized to obtain the effective properties of the laminate in a second homogenization step. The latter is beneficial when large composite components have to be simulated and ply failure can be excluded.

The procedure is exemplified for laminates consisting of glass fiber reinforced polyester resin for which the matrix data is determined from dynamic mechanical analysis (DMA) tests and the fiber data is taken from literature. The linear viscoelastic properties of UD plies, random fiber plies, and laminates with different layups are predicted and the outcomes are compared with corresponding DMA experiments.

The funding of the Polymer Competence Center Leoben GmbH (PCCL) within the COMET-program by the Austrian Federal Ministry for Transport, Innovation and Technology (BM-VIT), the Austrian Federal Ministry of Digital and Economic Affairs (BMDW), Österreichische Forschungsförderungsgesellschaft mbH (FFG), the Provinces of Styria, Lower Austria and Upper Austria is gratefully acknowledged.

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A constitutive model for fiber reinforced polymer plies - transition from hardening to softening behavior during anisotropic damage evolution

Jan Kaul (*TU Wien, Austria*)

14:20

Heinz E. Pettermann (*TU Wien, Austria*)

In the present work an extension to the damage formulation for the constitutive model for fiber reinforced polymers, proposed in [1], is presented. The existing model predicts plastic strain accumulation and uses continuum damage mechanics to model the stiffness degradation accompanied by strain hardening as well as strain softening behavior. In contrast to the majority of constitutive models for FRP plies, the damage evolution for the hardening behavior is formulated in terms of stresses. On one hand, this enables the use of well established fracture criteria, but on the other hand it poses difficulties combining the formulation for hardening with one for softening in a unified manner. Firstly, this is due the fact that the damage variables cannot be described as injective functions in terms of the stresses for both hardening and softening. And secondly, this is due to the fact that the softening behavior has to be mesh-adjusted, while the hardening has not. To overcome these difficulties, a piecewise formulation is used in [1], with a damage evolution law based on the Puck fracture criterion for the hardening and a damage evolution law based on equivalent strains for the softening behavior.

The aim of the present work is to unify the formulation by employing the framework presented in [2], where the damage evolution is controlled by a set of loading threshold functions. To identify critical states for the transition from hardening to softening, for multiple evolving internal damage variables, a transition condition is introduced. Furthermore the softening branches of the loading threshold functions are adjusted to provide meshsize-independent results. The extension to the constitutive model as well as the consistent Jacobian are implemented in a material subroutine for ABAQUS/Standard (SIMULIA, Providence, RI, USA).

The capabilities of the proposed damage formulation are demonstrated on various angle-ply laminates. The transition from hardening to softening is studied by using laminates with different ply angles to intentionally induce different levels of strain hardening before the onset of softening. References:

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An anisotropic creep model for continuously and discontinuously fiber reinforced materials

Sascha Fliegner (*Fraunhofer-Institut für Werkstoffmechanik IWM, Germany*)

14:40

Jörg Hohe (*Fraunhofer-Institut für Werkstoffmechanik IWM, Germany*)

Fiber reinforced composite materials are important materials in lightweight construction. In contrast to aerospace components or wind turbine blades with limited numbers of components to be manufactured, especially the automotive sector is characterized by industrial scale mass production with large numbers of components to be manufactured with an extreme demand for short cycle times. For this purpose, polymeric composite and sandwich components consisting of thermoplastic base materials are promising candidates for future composite automotive designs. On the other hand, one of the major shortcomings of thermoplastic composites is the distinct tendency of thermoplastic polymers towards creep due to the limited crosslinking of their macromolecules. The present study is concerned with the formulation, implementation and validation of anisotropic creep laws for neat thermoplastic matrix materials, discontinuously long fiber reinforced thermoplastic (LFT) composite materials with process dependent fiber preference directions as well as unidirectionally fiber reinforced thermoplastic tapes. Based on a simple three parameter Kelvin-Voigt approach, an anisotropic model is formulated and implemented into a finite element program. The model is validated against an experimental data base of creep experiments on LFT materials and unidirectionally continuously fiber reinforced specimens. In

addition, the model is applied in its isotropic version to a multiscale analysis and homogenization of a random long fiber reinforced material. In order to validate the model further, breadboard structures consisting of sandwich panels with thermoplastic laminates as face sheets featuring local LFT functionalizations are tested under long term static loading conditions in the creep regime. The experimental results are found in a rather good agreement with a finite element prediction of the creep response of the considered breadboards.

FEM-simulation of the mechanical behavior of woven fabric composites using an anisotropic hyperelastic material model

Monika Gille (*Deutsches Institut für Kautschuktechnologie e.V., Germany*) 15:00

Nils Hendrik Kröger (*Deutsches Institut für Kautschuktechnologie e.V., Germany*)

Daniel Juhre (*Otto-von-Guericke University, Magdeburg*)

Woven fabric composites are being widely used in technical fields such as automotive industry and aviation. The correct description of the material behavior by suitable material models is important for the prediction of the mechanical properties of composite components using the finite element method (FEM). The deformation behavior of an elastomeric test specimen with an embedded fabric is investigated. Despite the symmetrical structure of the individual fabric yarns in the form of a plain weave, the fabric shows a pronounced directional dependence. This directionality is conditioned by the manufacturing process.

As a model assumption, the bonding between elastomer-matrix and fabric is considered to be ideally adhesive. To simplify the structure of the composite it is divided into two kinds of layers. It consists of an elastomer layer and a homogenized layer for the woven fabric. The interface between elastomer and fabric is idealized. Thus, there are also areas containing rubber in the fabric layer. The material behavior of the elastomer layers are modeled with the MORPH model (Model Of Rubber PHenomenolgy) using the concept of representative directions for 3D implementation. For the modeling of the anisotropic fabric layer and the simultaneous presence of high deformations, an anisotropic hyperelastic material model is used.

The parameters of the anisotropic hyperelastic material model are adjusted by means of tension and shear tests on the fabric and the composite itself. As validation a bending test of the material is performed and simulated.

Parameter identification for constitutive models of innovative textile composite materials using digital image correlation

Justin Felix Hofmann (*University of Kassel, Germany*) 15:20

Claudia von Boyneburgk (*University of Kassel, Germany*)

Sophie Tunger (*University of Kassel, Germany*)

Hans-Peter Heim (*University of Kassel, Germany*)

Detlef Kuhl (*University of Kassel, Germany*)

This contribution focuses on an innovative composite material consisting of textile layers made from continuous wooden fibers embedded in a polymer matrix. A finite element simulation of potential use-cases is planned to aid the development process and to assess the suitability of the material in an architectural context. The simulation is based on a constitutive model assuming homogenous orthotropic elastic behavior and will be expanded to include multiscale modeling in future research. The material parameters used in such models can often be determined based on local measurements during comparatively simple experiments (e.g. tensile tests) which assume homogenous stress and strain distributions at least in large parts of the specimen. However, this is not always the case, especially when dealing with non-isotropic materials in off-axis configurations and the need for full-field measurements like digital image correlation (DIC) arises.

Experimental results of uniaxial on- and off-axis tensile tests using DIC are presented and used in the identification of the material parameters of the given model. Results of simulations and experiments are compared and the suitability of the material model is discussed.

Characterization of fiber matrix interface of continuous-discontinuous fiber reinforced polymers on the microscale

Benedikt Rohrmüller (*Karlsruher Institut für Technologie (KIT), Germany, Fraunhofer-Institute for Mechanics of Materials IWM, Germany*) 15:40

Michael Schober (*Karlsruher Institut für Technologie (KIT), Germany, Fraunhofer-Institute for Mechanics of Materials IWM, Germany*)

Kerstin Dittmann (*Fraunhofer-Institute for Mechanics of Materials IWM, Germany*)

Peter Gumbsch (*Karlsruher Institut für Technologie (KIT), Germany, Fraunhofer-Institute for Mechanics of Materials IWM, Germany*)

Jörg Hohe (*Fraunhofer-Institute for Mechanics of Materials IWM, Germany*)

Fiber reinforced polymers are an important material group in lightweight constructions. Therefore a thorough knowledge of the material properties of fibers, matrix and the connecting interfaces plays an important role in the further development of simulation models. The goal of this work is especially to characterize the fiber matrix interface. Because it is difficult to get detailed information on crack initiation and propagation on the macroscale, tensile tests with in-situ observation are carried out on the microscale. The micro specimens which are prepared out of compression molded plates of sheet molding compound (SMC) have a gauge length of approx. 1 mm. Via a microscope and digital image correlation, one specimen surface side is traced and evaluated. For the modeling, finite element simulations are conducted. In the elastic range some homogenization approaches are tested and compared to the measurement results.

S06.05 | Material modelling in solid mechanics

Date: February 20, 2019
Room: SR 05

14:00-16:00

An analytical study on the role of misfit dislocations in fracture toughness enhancement of superlattice coatings

Antonia Wagner (*TU Wien, Austria*) 14:00

David Holec (*Montanuniversität Leoben, Austria*)

Melanie Todt (*TU Wien, Austria*)

Paul Heinz Mayrhofer (*TU Wien, Austria*)

Matthias Bartosik (*TU Wien, Austria*)

Coherently grown multilayer coatings with a periodicity length in the nanometer range exhibit a superlattice (SL) effect in mechanical properties like hardness and fracture toughness. A strong dependency of this enhancement on the bi-layer period has been shown in [1, 2]. The superlattice effect in hardness is well described by the model after Chu and Barnett [3] based on dislocation glide across and within the layers. However, the fracture toughness enhancement derived from experiments showing brittle fracture must be a consequence of a bilayer-period-dependent mechanism active in the absence of plastic deformations. One of these mechanisms might be the residual stress state after the manufacturing process, which will be discussed in this study.

We can distinguish between extrinsic residual stresses due to a mismatch of the coefficients of thermal expansion and intrinsic stresses originating from the film growth process. A major part

of the latter originates from the epitaxial growth of the coating and a lattice mismatch of its constituents leading to coherency stresses. Up to a critical thickness of the layers this mismatch is accommodated by elastic strain, thereafter misfit dislocations form [4, 5].

The analytical model developed within this study is based on the Euler-Bernoulli beam theory applied to an inhomogeneous beam in conjunction with an overall energy balance. Considering the energy necessary for a dislocation to form and the strain energy of the substrate-coating system, a certain dislocation density can be calculated for each layer depending on its thickness. Modelling a layer-by-layer growth including misfit dislocations, the residual stress state of superlattice systems is predicted as a function of the bilayer period.

Finally, the analytically estimated residual stresses are used to predict the apparent fracture toughness and its dependence on the bilayer period of respective SL architectures, considering the intrinsic fracture toughness of the phases and the spatial variation of elastic properties.

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A framework and finite element formulation for incompatibility tensor-based gradient plasticity

Tobias Kaiser (*TU Dortmund University, Germany*)

14:20

Andreas Menzel (*TU Dortmund University, Germany, Lund University, Sweden*)

In this contribution we present a thermodynamic consistent approach to account for the action of geometrically necessary dislocations in finite strain plasticity as an extension to purely phenomenological approaches to model strain hardening. The theory proposed relies on an extended form of the dissipation inequality by a so-called nonlocality residual (*Eur. J. Mech. A/Solids*, 17 (1998), 741-761) which effectively induces a nonlocal character to the dissipation inequality. Since nonlocal theories are, in general, difficult to handle due to the evaluation of integrals, we focus on a special choice of the introduced regularisation operator which results in a gradient plasticity formulation. Evaluating the nonlocal format of the dissipation inequality for an energy function which takes into account a dislocation density tensor gives rise to the balance equation of a stress field which takes the interpretation of a back-stress tensor in the yield function based on energetic dualities.

Elaborating a specific model, we present finite element based simulation results which rely on the solution of the plastic consistency conditions by means of Fischer-Burmeister complementary functions on a global level. We show that the model is capable of reproducing shear bands of finite width that are induced by geometric imperfections in softening materials and discuss the model properties at material interfaces where the plastic variables exhibit jump-discontinuities.

Thermodynamic dislocation theory: torsion of bars

Yinguang Piao (*Ruhr University Bochum, Germany*)

14:40

Khanh Chau Le (*Ruhr University Bochum, Germany*)

The thermodynamic dislocation theory (TDT), originally developed by Langer, Bouchbinder, and Lookman [*Acta Mat.* 58, 3718(2010)], deals with the uniform plastic deformations of crystals,

which can only have redundant dislocations with vanishing resultant Burgers vector. For non-uniform plastic deformation, such as torsion of bars and bending of beams, there exist excess dislocations in order to fulfill the incompatibility conditions. At first glance, the TDT is not applicable to these problems due to the absence of excess dislocations. However, it turns out that the density of excess dislocations for bars of macro sizes under torsion with small to moderate twist angles is negligibly small. Therefore, for such bars a simple extension of the TDT proposed in this work that takes into account the spatial variation of state variables while ignoring the excess dislocations is possible. This extension is expressed by a coupled system of equations of motion for the flow stress, dislocation density as well as its entropy. Employing a small set of physics-based parameters, which we expect to be approximately independent of strain rate and temperature, we are able to simulate the torque-twist curve for a bar made of single crystal copper. With the same physics-based parameters and different initial parameters of the sample, our simulations agree well with torque-twist curves of two samples in the experiment.

Thermodynamic dislocation theory of adiabatic shear banding in steel

Tuan Minh Tran (*Ruhr University Bochum, Germany*)

15:00

Khanh Chau Le (*Ruhr University Bochum, Germany*)

J.S. Langer (*University of California, USA*)

The statistical-thermodynamic dislocation theory developed in our earlier studies is used here in an analysis of the experimental observations of adiabatic shear banding (ASB) in steel by Marchand and Duffy (1988). These scientists made stress-strain measurements over a range of substantially different temperatures and shear rates using thin steel tubes bonded to torsional Kolsky bars. They observed ASB formation at high shear rates and low temperatures. Specifically, they observed abrupt stress drops, large increases of temperature in emerging narrow bands, and strong strain localization leading to crack formation and failure. Our challenge is to predict those behaviors quantitatively employing a small set of physics-based parameters, which we expect to be approximately independent of strain rate and temperature, and in this way to obtain additional information about the properties of structural materials. We make a simple model of a weak notch-like disturbance that, when driven hard enough, triggers shear banding instabilities that are quantitatively comparable with those seen in the experiments.

Thermodynamic dislocation theory

Khanh Chau Le (*Ruhr-Universitaet Bochum, Germany*)

15:20

This paper proposes the thermodynamic dislocation theory for uniform and non-uniform plastic deformations which takes into account the effective disorder temperature. We use it to simulate the stress-strain curves for crystals that are subjected to simple shear, tension/compression, and torsion tests. We show the size and the Bauschinger effects due to the excess dislocations, as well as the strain rate and the thermal effects due to the redundant dislocations and disorder temperature. Finally, we make a simple model of a weak notch-like disturbance that, when driven hard enough, triggers shear banding instabilities that are quantitatively comparable to those of Marchand and Duffy's experiments.

Leaving the slip system - cross slip in continuum dislocation dynamics

Benedikt Weger (*Graz University of Technology, Austria*)

15:40

Thomas Hochrainer (*Graz University of Technology, Austria*)

Dislocations are the main contributors to plastic deformation of crystalline materials. An important step towards the description of hardening behavior is the implementation of cross slip, as it is

the main contributor for the exchange of dislocations between various slip systems. Furthermore, it plays a major role in the description of further dislocation reactions, such as multiplication or annihilation.

In conventional density based continuum-mechanical theories of dislocations, dislocations are considered closed curves which cannot end inside the crystal. Recent discrete dislocation dynamics simulations suggest that only a small fraction of dislocations is actually closed on a single slip system. Hence, the idea of describing dislocations as open curves within each slip systems seems reasonable. A global constraint can guarantee the overall closure of all dislocation lines.

The assumption of open curves leads to modified evolution equations for the state variables of higher dimensional continuum dislocation dynamics. Projecting the state variables on the three dimensional euclidean space leads to a description of cross glide with only a few internal state variables per slip system.

The resulting equations are checked for plausibility by numerical calculations with various initial conditions. The exchange of state variables between two slip systems is implemented into the crystal plasticity framework DAMASK.

S06.06 | Material modelling in solid mechanics

Date: February 20, 2019

16:30-18:30

Room: BIG HS

Constitutive modelling of woven fiber reinforced polymer

Sophie Tunger (*University of Kassel, Germany*)

16:30

Zuardin Akbar (*University of Kassel, Germany*)

Justin Felix Hofmann (*University of Kassel, Germany*)

Philipp Eversmann (*University of Kassel, Germany*)

Detlef Kuhl (*University of Kassel, Germany*)

Nowadays the application of renewable resources becomes more and more the focus of attention in architecture and civil engineering. Therefore, new sustainable materials are developed, and the understanding of their constitutive behavior is of high relevance.

In this contribution, a fiber reinforced composite material is considered. The different constituents of the heterogeneous material are a polymer matrix and layers made of wooden continuous fibers. Since the fibers are not unidirectional but woven, the material behavior is anisotropic and non-linear.

On the macroscopic length scale the homogenized material can be considered as nearly orthotropic because of the small bending of the fibers. Based on experimental data a phenomenological macroscopic material model is developed. The correlation of stresses and strains can be modelled by different approaches. A short overview of the concepts for modeling orthotropic material behavior on the macroscopic level will be given.

With the behavior of the macroscopic structure being influenced by its microscopic structure, a multiscale approach is taken into account. A FE² - concept will be shown to compute the overall behavior.

Multiscale modeling and optimization of braid-reinforced polymer coil springs

Marc Luger (*University of Innsbruck, Austria*)

16:50

Roland Traxl (*University of Innsbruck, Austria*)

Ulrich Hofer (*University of Innsbruck, Austria*)

Benjamin Hirzinger (*University of Innsbruck, Austria*)

Roman Lackner (*University of Innsbruck, Austria*)

Purposive custom-tailoring of laminated textile-reinforced polymers demands reliable simulative frameworks to predict the individual reinforcement layers' structural response, yielding potential of optimization of structural components' mechanical performance.

Multiscale modeling is standardly employed to obtain the effective (homogenized) elastic properties of composites, whereas both analytical and numerical upscaling methods are commonly applied. Whilst analytical methods of elastic homogenization usually cause low computational expenses, little information is gained concerning the stress and strain situation as well as the mechanical out-of-plane behavior. As regards numerical methods, FE-based unit cells are standardly employed to predict the elastic behavior of yarns or braided reinforcement layers within the composite.

Within the presented multiscale method [Luger et al. 2018], a modeling approach employing 3D continuum models to overcome the aforementioned shortcomings is proposed. Hereby, attempting to reduce the number of parameters, idealized geometric properties are employed for the observation scales' numerical representations.

Starting from the definition of observation scales - the yarn, the braid, and the component scale -upscaling procedures are employed to obtain effective properties at each scale, whereas the properties of the constituents, i.e. fiber and matrix, serve as input for multiscale modeling:

At yarn scale, suitable geometric fiber arrays are employed within these FE-models to obtain effective elastic yarn properties. Besides the aforementioned constituent materials, awareness of applicable fiber-volume-ratio is mandatory.

At braid scale, FE-based unit-cells are employed to obtain the effective elastic braid properties, applying the effective yarn properties, and matrix properties describing the resin pockets. The influence of geometric braid properties such as braid angles, braid patterns, and yarn undulations is reflected within the geometric arrangement of the FE model.

At component scale, the effective braid properties are employed within structural simulations to assess the component's mechanical performance, rendering prospects for purposive optimization. In order to assess the predictive capabilities of the proposed multiscale model, the experimentally determined structural response of coil springs, consisting of glass-fiber-reinforced epoxy, is compared to numerical results obtained from the proposed method by employing the subsequent upscaling. Effective braid properties are hereby applied to a suitable FE representation of the spring at component scale, accounting for the local geometric braid characteristics, e.g. curvature-induced variation of the braid angle.

References

[Luger et al. 2018] Luger, M., Traxl, R., Hofer, U., Hirzinger, B., Lackner, R. (2018). RUC-based multi-scale model for braid-reinforced polymers: Application to coil springs. *Composites Part B: Engineering* 155 (2018): 431-443.

Multiscale modeling of viscoelastic behavior of braid-reinforced polymer components

Ulrich Hofer (*University of Innsbruck, Austria*)

17:10

Marc Luger (*University of Innsbruck, Austria*)

Roland Traxl (*University of Innsbruck, Austria*)

Roman Lackner (*University of Innsbruck, Austria*)

Multiscale modeling is standardly employed to obtain the effective (homogenized) physical properties of composites, whereas both analytical and numerical upscaling methods are commonly applied. As regards effective viscoelastic properties, analytical methods are often obtained by extending their elastic counterparts to viscoelasticity by exploiting the so-called correspondence principle. As regards numerical methods, FE-based unit cells are standardly employed to determine the viscoelastic behavior of composites.

Within the presented multiscale method, fractional viscoelastic models are used to describe the time-dependent behavior of the matrix, well-capturing the experimentally observed viscoelastic behavior with a comparatively low number of parameters. At three observation scales - the yarn scale, the braid scale and the component scale [Luger et al. 2018] - upscaling methods are introduced to obtain effective viscoelastic properties at each scale, whereas the properties of the constituents, i.e. fiber and matrix, serve as input for multiscale modeling:

- At yarn scale, the Chamis-equations - standardly used for predicting the effective elastic properties of unidirectionally-reinforced composites - are extended towards viscoelasticity by employing the aforementioned correspondence principle. Hereby, the viscoelastic homogenization problem is transformed into the Laplace-Carson domain, where the corresponding elastic problem is solved. An inverse Laplace-Carson transformation gives closed-form expressions for the effective viscoelastic properties of the yarns [Hofer et al. 2018].
- At braid scale, the upscaling strategy described in [Luger et al. 2018] is extended towards viscoelastic behavior. By doing so, FE-based unit cells are employed to obtain the effective viscoelastic braid properties, applying the effective yarn properties as obtained by the extended Chamis-equations and considering the influence of geometric braid properties, such as the braid angle.
- At the component scale, the effective braid-properties are employed within structural simulations to obtain the viscoelastic response of braid-reinforced components.

In order to assess the quality of the multiscale model, compressional creep tests on braid-reinforced tubes are performed. The model results agree well with the experimentally-obtained results. Moreover, the experimentally-observed influence of the braid geometry onto the viscoelastic behavior is well reproduced by the proposed multiscale method.

References

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Orthotropic hyperelastic energy functions for the geometrically nonlinear simulation of textile membrane structures

Mehran Motevalli (*Ruhr Universität Bochum, Germany*)

17:30

Jörg Uhlemann (*Universität Duisburg-Essen, Germany*)

Natalie Stranghöner (*Universität Duisburg-Essen, Germany*)

Daniel Balzani (*Ruhr Universität Bochum, Germany*)

New hyperelastic orthotropic material formulations are proposed for the simulation of textile membranes. Part of the models is polyconvex and thus, a physically meaningful and mathematically robust formulation is obtained. The models are adjusted to the stress-strain paths of a glass-PTFE fabric under cyclic uniaxial and biaxial tension tests in warp and fill direction. From the experiments it is shown that an elastic response can not yet be reached within only 3 to 5 load cycles, which however is standard procedure in practical engineering. In contrast to this, here the number of cyclic loads is increased to 20 load cycles. Unlike the common adjustment procedure for a linear elastic orthotropic model, the lateral contraction of the uniaxial tension tests is not neglected here and thereby, the model may capture the strong crosswise interaction between the warp and fill yarns with the utilized orthotropic terms. It is shown that a linear elastic model

can not sufficiently represent this complex behavior and even a hyperelastic model with a simple superposition of purely transversely isotropic energies for the warp and fill directions also fails to qualitatively describe this response. Moreover, a new large scale experimental setup is presented which enables the investigation of the material response in a structural problem. The adjusted material model is implemented to simulate the material response of the membrane in this new test setup. The response of the proposed models is compared with the standard linear elastic model. Furthermore, the new models are compared to each other with respect to their precision to represent the experimental data and with regard to the mathematical characteristics as well as their robustness in numerical simulations.

Invariant formulation of anisotropic plasticity for fiber-reinforced composites: rate-type models with anisotropic, non-linear kinematic hardening

Swaroop Gaddikere Nagaraja (*Montanuniversitaet Leoben, Austria*)

17:50

Martin Pletz (*Montanuniversitaet Leoben, Austria*)

Clara Schuecker (*Montanuniversitaet Leoben, Austria*)

The use of fiber-reinforced composites as a primary structural component in automotive and aerospace industries has significantly increased over time, due to their great weight saving potential. Therefore, the predictive modeling of the non-linear behavior of composites has been a topic of intensive research over the last years. From an experimental perspective, investigations pertaining to the nonlinear behavior of composites are documented in [1]. These non-linearities are strongly influenced by the matrix(polymer), which is plasticized at relatively small deformations, in contrast to fibers(carbon) that remain essentially elastic up to failure.

This study presents a sufficiently general, homogenized formulation of anisotropic elastoplasticity for application to unidirectional fiber-reinforced composites. Two constitutive models have been developed to simulate the non-linearities exhibited by the composite, generating the anisotropic elastic and plastic response functions with the aid of representation theory. Rate-independent versions using isotropic hardening have been proposed in [2]. In the present work, the models are extended to include rate dependency and non-linear kinematic hardening effects. Selected numerical simulations which serve the purpose of evaluating the models qualitatively and quantitatively are presented at the end.

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S06.07 | Material modelling in solid mechanics

Date: February 20, 2019

16:30-18:30

Room: SR 05

Modelling ductile damage and fracture in extrusion-formed thin-walled aluminium components

Sandra Baltic (*Materials Center Leoben, Austria*)

16:30

René Hammer (*Materials Center Leoben, Austria*)

Julien Magnien (*Materials Center Leoben, Austria*)

Thomas Antretter (*Montanuniversität Leoben, Austria*)

Although modelling damage evolution and ductile fracture are mature fields of research, many details remain to be tackled for reliable predictions in real scale models. As reported by Cao et al. (2015), both phenomenological and micromechanical models can predict the location of maximum damage. However, prediction of the instant of fracture is still an open question. Damage formulations must imply variables characterizing different stress states in order to obtain realistic results for complex loading paths.

The object of our research is to model the ductile behaviour of an aluminium alloy A-1050 formed into a can by impact extrusion, and subsequently exposed to high internal pressure. For safe pressure handling, a rupture point, i.e., a safety vent is designed. Various sample geometries are cut out from the aluminium cans to characterize different states of stress and to construct a well-defined fracture locus. Experiments have shown that the structural response of the material is accompanied by softening and strain localization. This motivates the development of a numerical model taking into account softening driven by accumulation of damage.

A complete procedure for characterization and modelling of a thin metal sheet is presented, resulting in a unique numerical formulation able to cover different stress states. A phenomenological ductile fracture model that involves parameters describing the stress state (stress triaxiality and Lode parameter) is coupled with plasticity and implemented in the FEM software ANSYS Mechanical APDL. A new coupling function is introduced capable of reproducing the diffuse and localized damage stage. The accumulation of damage D , dictated by the current stress state, drives the softening process.

The pertaining material parameters are calibrated explicitly from conventional tensile tests. For validation, a FEM simulation of the aluminium can under a real loading scenario is performed. The numerical results are compared with the evidence found in pressure tests of the cans. It is shown that the mechanical response of extruded aluminium cans is predicted accurately. The simulation thus enables a reliable safety vent design ensuring safe pressure handling.

References

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A comparison between the performance of different Mindlin's theory based strain gradient models in local singularities

Resam Makvandi (*Otto von Guericke University Magdeburg, Germany*)

16:50

Daniel Juhre (*Otto von Guericke University Magdeburg, Germany*)

The classical continuum mechanics theories are originally supposed to determine deformations in ranges from millimeter to meter, the so-called macroscopic scales. In fact, these models

are approximations of physical systems neglecting the underlying microstructure. For instance, a Cauchy continuum, i.e. a continuum with an elastic energy determined as a function of the gradients of its macroscopic displacement, can only approximate the behavior of a physical system sufficiently as long as the microstructure has a much smaller length-scale than the macrostructure [1]. Although these models were exploited in studies for large and small scales, experiments have shown that the classical models are not able to properly cover the smaller scales; In particular, problems in micron- and nano-dimensions are frequently observed. Size-effects, which cannot be captured exploiting these theories, seem to be the source of this issue. On top of that, the appearance of local singularities at the crack tips (or more broadly, in the presence of point and line loads) is one of the known limitations of the classical continuum mechanics theory. Generalizing these models by introducing additional kinematic terms to consider the underlying microstructure effects at macroscopic levels is one way of overcoming the already mentioned problems.

In this contribution, we will focus on the Mindlin's theory of elasticity with microstructures and its different forms. Therein, it is shown that for the first strain gradient theory, five additional parameters must be introduced. However, in practice, due to the complexities of measuring the new parameters, various simplified versions of the theory are being exploited, among them we name Altan et al. [2] and Reiher et al. [3]. Our aim here is to compare the performance of these simplified theories in removing the local singularities of the conventional continuum mechanics theory.

References:

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- [2] S.B. Altan, E.C. Aifantis, On the structure of the mode III crack-tip in gradient elasticity, *Scripta Metallurgica et Materialia* 26 (2) (1992) 319-324.
- [3] Reiher Jörg Christian, Giorgio Ivan, Bertram Albrecht, Finite-Element Analysis of Polyhedra under Point and Line Forces in Second-Strain Gradient Elasticity, *Journal of Engineering Mechanics* 143 (2) (2017) 4016112.

A new anisotropic hyperelastic material model for single layer blue phosphorus

Farzad Shirazian (*RWTH Aachen University, Germany*)

17:10

Reza Ghaffari (*RWTH Aachen University, Germany*)

Ming Hu (*University of South Carolina, USA*)

Roger A. Sauer (*RWTH Aachen University, Germany*)

Here, a new hyperelastic material model for single layer blue phosphorus is presented. It is non-linear and can capture anisotropic behavior of the material. The strain energy density is written in terms of a set of invariants. These invariants are based on the logarithmic strain and structural tensor [4]. The constitutive laws have a periodicity of 60 degrees that is reproduced with the structural tensor. A set of virtual tests, two perpendicular uniaxial stretches and one pure dilatation, is designed for calibration of the model. The virtual tests are done using density functional theory as implemented in the Quantum ESPRESSO package. An ultrasoft pseudopotential and a GGA exchange-correlation functional is used in the ab-initio simulations. The model is then implemented in the rotation-free shell formulation of [5] which is based on curvilinear coordinates and isogeometric finite elements. Finally, Indentation of a blue phosphorus sheet is simulated using the new formulation.

Previously, the employed framework was used for development of membrane and shell material models for graphene [1, 2, 3].

References

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- [2] Reza Ghaffari, Thang X. Duong, and Roger A. Sauer. A new shell formulation for graphene structures based on existing ab-initio data. Int. J. Solids Struct., 135:37-60, 2018.
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- [4] Q.-S. Zheng. Two-dimensional tensor function representation for all kinds of material symmetry. Proc. R. Soc. A, 443(1917):127-138, 1993.
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Prandtl-Reuss model without safe-load conditions

Konrad Tomasz Kisiel (*Warsaw University of Technology, Poland*)

17:30

We will discuss the existence theory to the well-known Prandtl-Reuss model of elasto-perfect plasticity. For a given body Ω and applied forces, the aim of the model is to find:

the displacement vector field $u : \Omega \times (0, T) \rightarrow R^3$,

the inelastic deformation tensor $e^\rho : \Omega \times (0, T) \rightarrow S_3 :=$ symmetric matrices $R^{3 \times 3}$.

For the Prandtl-Reuss model it is assumed that the inelastic constitutive equation which describes e^ρ is given by a differential inclusion, where the right hand side is the subgradient of the indicator function of the set of admissible stresses K .

Since 80's (R. Temam, G. Anzellotti, S. Luckhaus) it is well known that if one assume so-called safe-load conditions then it is possible to obtain a solution (u, e^ρ) such that inelastic constitutive equation is satisfied in the sense of measures. However, safe-load conditions are very difficult to check in applications. Therefore, the natural question is: If safe-load conditions are necessary to obtain the existence of a solution to the Prandtl-Reuss model of elasto-perfect plasticity?

The main purpose of this talk is to answer this question. Namely, we were able to prove that, if applied force (Neumann boundary data) is not too large (upper bound depends on the set of admissible stresses K), then there is no need to use any type of safe-load conditions.

The talk is based on methods and results presented in:

[1] K. Kisiel. Dynamical poroplasticity model - existence theory for gradient type nonlinearities with lipschitz perturbations. J. Math. Anal. Appl., 450(1):544-577, 2017.

[2] K. Kisiel and K. Chelmiński. Prandtl-reuss model of elasto-perfect plasticity without safe-load conditions. under review.

Automatic analysis of the stress-strain response of rheological models

Timm Schultz (*Technische Universität Kaiserslautern, Germany*)

17:50

Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

Viscoelastic material behaviour can be represented by rheological models combining elastic and viscous rheological elements. These combinations of elastic springs and viscous dashpots can be simple as the well known Maxwell model consisting of only one spring and one dashpot, more complex like the four element Burgers model or very complex consisting of several elements combined in various ways.

An Algorithm is presented allowing the calculation of stress and strain of a viscoelastic rheological model in response to a given input signal in a simple and effective way. Such a model can

be a system consisting of an arbitrary number of rheological elements. This is achieved by the formulation of transfer functions for basic rheological elements based on their constitutive equations and using the Laplace transform. Transfer functions of element combinations and systems of rheological elements can be derived from these basic functions allowing the calculation of the stress or strain response of entire systems, subsystems and single elements due to a given input signal.

The method of analysing a system by the use of transfer functions originated in system theory and best known from the field of electrical engineering works well for linear time-invariant transmission systems. As many materials show a nonlinear material behaviour a method for calculating the response of a system including nonlinear elements to a given input signal is developed. To do so methods used in feedback control systems and nonlinear system analysis are investigated.

S06.08 | Material modelling in solid mechanics

Date: February 21, 2019

08:30-10:30

Room: BIG HS

Strain induced crystallization and fracture of rubber-like materials

Christian Linder (*Stanford University, United States of America*)

08:30

Reza Rastak (*Stanford University, United States of America*)

Prajwal Kammardi Arunachala (*Stanford University, United States of America*)

A multi-scale polymer network model is proposed for strain-induced crystallization phenomena in rubber-like materials [1] and extended to account for phase field fracture. At the microscopic scale, the thermodynamic behavior of a polymer chain inside a stretching polymer network and its crystallization is studied and a new polymer chain model is presented. The chain model accounts for the thermodynamics of crystallization and presents a rate-dependent evolution law for crystallization based on the gradient of the free energy with respect to the crystallinity variable to ensure the dissipation is always non-negative. The multiscale framework allows anisotropic crystallization of rubber which has been observed experimentally. Two different approaches for formulating the orientational distribution of crystallinity are studied. For the discrete distribution, crystallization is tracked at a finite number of orientations. On the other hand, the continuous distribution captures the anisotropic behavior with only a few distribution parameters. To connect the deformation of the micro with the macro scale, the recently developed maximal advance path constraint is combined with the principle of minimum free energy, resulting in a non-affine deformation model for polymer chains. The model is then combined with a phase field approach to fracture. Various aspects of the proposed model are validated by existing experimental results, including the stress response, crystallinity evolution, crystallinity distribution, the rotation of the principle crystallization direction, and the effect on the fracture behavior of rubber-like materials.

References:

[1] Rastak, R., Linder, C., "A non-affine micro-macro approach to strain-crystallizing rubber-like materials" *Journal of the Mechanics and Physics of Solids*, 111, 67-99 (2018).

Hyperelastic modelling and experimental characterisation of cellular rubber

Alexander Ricker (*Deutsches Institut für Kautschuktechnologie e.V., Germany*)

08:50

Nils Hendrik Kröger (*Deutsches Institut für Kautschuktechnologie e.V., Germany*)

Marvin Ludwig (*Toyoda Gosei Meteor GmbH, Germany*)

Ralf Landgraf (*Technische Universität Chemnitz, Germany*)

Jörn Ihlemann (*Technische Universität Chemnitz, Germany*)

Cellular rubbers are elastomeric materials containing pores. Those rubbers can undergo large volumetric deformations. They are widely-used in seals, weather stripping and vibration damping applications.

This paper presents an isotropic, hyperelastic material model using the approach of Danielsson et al. The constitutive equations are derived from the kinematics of an idealized pore, represented by an incompressible hollow sphere distorted to an ellipsoid. Homogenising the elastic strain energy of the matrix material leads to an energy potential describing the cellular rubber behaviour. The approach is extended by adding higher order terms, which requires a three-dimensional numerical integration. This is realised by combining a spherical Lebedev-quadrature with a radial Gauss-quadrature. In addition, pore pressure is considered under the assumption of ideal gas behaviour. The model is implemented into the finite element software MSC Marc. Moreover, a feasible procedure of parameter fitting avoiding lateral strain measurement is outlined and tested.

For model validation and parameter fitting, experimental characterisations were carried out on four foamed elastomers and the corresponding pore-free materials. The digital image correlation technique is used to obtain experimental data of the lateral contraction behaviour of the elastomers under uniaxial tension. The FE implementation is demonstrated by simulating a compression test on a car door seal.

Application of different plasticity models to PC/ABS blends within a micromechanical unit cell approach

Jonas Hund (*Karlsruhe Institute of Technology (KIT), Germany*)

09:10

Thomas Seelig (*Karlsruhe Institute of Technology (KIT), Germany*)

Rubber-toughened thermoplastic polymer blends of polycarbonate (PC) and acrylonitrile butadiene styrene (ABS) are available in various compositions for many applications. Key microstructural parameters are the PC vs. ABS ratio and the rubber content of ABS. PC/ABS blends exhibit a pronounced plastic dilatancy in their overall deformation behavior. This volume increase results from different damage mechanisms (void growth, crazing) which prevail primarily in the ABS phase, e.g. [1].

In this work, unit cell models based on micrographs are used to model PC/ABS blends of various compositions. Therein, each phase (PC, ABS) is represented by appropriate material models accounting for the finite strain viscoplastic behavior. Special emphasis is put on the modeling of the ABS phase with its complex failure mechanisms. While different material models are well capable of capturing the deformation and failure behavior of ABS under uniaxial tension, reproducing the material's response under elevated stress triaxialities is still an issue. Several models which account (either phenomenologically or via a micromechanical approach) for the different failure mechanisms of ABS are compared. These models are used in finite element simulations of unit cell models of various compositions over a wide range of strain rates. Results regarding deformation and failure behavior are compared to experimental findings from the literature.

[1] Van der Giessen, E., Seelig, Th., 2015. Computational modeling of rubber-toughening in amorphous thermoplastic polymers - a review. *Int. J. Frac.* 196, 207-222

Experimental investigation, modelling and simulation of the DLO-effect using the example of thermo-oxidatively aged nitrile rubber

Bruno Musil (*Universität der Bundeswehr München, Germany*)

09:30

Michael Johlitz (*Universität der Bundeswehr München, Germany*)

Alexander Lion (*Universität der Bundeswehr München, Germany*)

Elastomers are used in almost all areas of industrial applications, such as tires, engine mounts, bridge bearings, seals or coatings. During their use in operation they are exposed to different environmental influences. These include in particular climatic factors such as air oxygen, high temperatures, light (UV radiation) and the influence of media (e.g. oils, fuels). A very important result of these factors is the chemical ageing of elastomers. In this case the elastomer degenerates and changes its chemical structure in the aged regions, which leads to an irreversible change of the material properties in connection with the reduction of its usability.

Here chemical ageing of Nitrile Butadiene Rubber (NBR) is investigated. Especially in case of thermo-oxidative ageing at elevated operating temperatures, ageing processes run inhomogeneous. These effects are known as diffusion-limited oxidation (DLO) and are associated with the diffusion-reaction behaviour of atmospheric oxygen with the elastomer network.

For these reasons, NBR samples are artificially aged in air and subjected to different experimental methods, which are presented and discussed. Further presented experimental results from inhomogeneous mechanical tests and permeation tests indicate the causes of the DLO-effect show the influence of chemical ageing and are subsequently used for parameter identification in relation to the diffusion-reaction equation.

A continuum mechanical modelling approach is also presented here, which describes the finite hyperelasticity, diffusion-reaction processes and chemical degradation and reformation of the elastomer network. This multifield problem results to a system of partial differential equations, evolution equations and constitutive equations and is solved within the Finite Element Method.

A phase field model for thermo-oxidative aging in cracked polymers

Jannik Voges (*Otto von Guericke University Magdeburg, Germany*)

09:50

Daniel Juhre (*Otto von Guericke University Magdeburg, Germany*)

When dealing with polymers, the behavior of aging processes is of great interest in many applications in engineering, as the usually very complex mechanisms can result in a drastic reduction of the lifetime of machine parts. In addition, those single mechanisms are coupled, which results in even more complexity. A crack creates new surfaces deeper inside the material and thus enables oxidation processes beyond the original surface. Once being oxidized, the crack resistance might be reduced, which may result in further crack propagation, which, again, enables oxidation even deeper.

In the present work, a new approach is introduced. The approach is based on the phase field method, which has become an important and versatile tool to model the evolution of materials. An evolution equation is underlain by a gradient energy term to capture an interface energy and by a second term which corresponds to the phase change representing the oxidation state. A diffusion equation controls the amount of available oxygen which is able to trigger the phase change. The phase change, in turn, drains a specific amount of oxygen in the coupled system of differential equations. In this work, cracks are able to engage the oxidation process deeper inside a specimen. Different numerical studies help to investigate the behavior of the model and are based on the finite element method.

Gibbs potential-based thermodynamics of rubber viscosity and viscoelasticity at large strains

Robert Plachy (*TU Wien - Vienna University of Technology, Austria*)

10:10

Stefan Scheiner (*TU Wien - Vienna University of Technology, Austria*)

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

During extrusion, rubber is subjected to large deformations including viscous and viscoelastic effects. Modeling approaches commonly applied for simulating rubber extrusion (such as Navier-Stokes equations, Newtonian, Bingham and Herschel-Bulkley models) have turned out to be not able to yield sufficiently accurate results. Furthermore, these approaches lack thermodynamic consistency, as they are not derived from an energy potential formulation, but being of a more or less heuristic nature.

Taking a step towards a possible solution of this unsatisfactory situation, Rajagopal et al. [Int J Eng Sci 70 (2013), 15-28] introduced a set of thermodynamically consistent, implicit material laws (e.g., for incompressible, anisotropic, and isotropic materials) based on the Gibbs potential (also called Gibbs free energy). Compared to the Helmholtz potential (also called Helmholtz free energy), which is usually formulated as a function of the (linearized) strain, the Gibbs potential is dependent on the stress state. Hence, the Gibbs potential does not require a reference to the initial configuration, as would be necessary in traditional large strain theory. However, while the above-cited and similar works or Rajagopal et al. are truly pioneering, some important aspects (such as large deformation theory, material derivatives, objectiveness) have remained unattended. Eradicating these deficits is the motivation of this contribution.

We start with a mass-related (instead of volume-related) formulation of the Gibbs potential. This way, the model is again freed from the need to link all volume elements (and thus the corresponding changes of their volumes) to the initial configuration, but rather allows for following the flow of a constant mass element. For that purpose, material derivatives and objective stress rates are introduced and included in the thermodynamic conservation laws. The objective stress rates are shown to be thermodynamically consistent, allowing for formulating the viscoelastic constitutive functions of large deformation flow processes, based on the Gibbs potential. Identification of material parameters for an isotropic (but time-dependent) compliance tensor related to rubber finally allows for predicting the deformation behavior of rubber when extruded through formative tools exhibiting simple shapes (such as circle or square).

The derived model is calibrated based on corresponding experimental data gained from specifically designed extrusion tests. The results of further, independent extrusion tests have been utilized for model validation; the latter has turned out as satisfying, corroborating the validity of this new approach to model the extrusion of rubber.

S06.09 | Material modelling in solid mechanics

Date: February 21, 2019

08:30-10:30

Room: SR 05

Computational modelling of inertia friction welding

Ross Albert Williams (*University of Glasgow, United Kingdom*)

08:30

Daniele Barbera (*University of Glasgow, United Kingdom*)

Andrew McBride (*University of Glasgow, United Kingdom*)

This study details the development and validation of a finite element methodology to robustly simulate the inertia friction welding (IFW) process. IFW allows for the welding of complex alloys and dissimilar materials not possible using conventional fusion processes. IFW is thus attractive to the aerospace sector for joining nickel superalloys. The process is driven by the frictional contact at the weldline where the temperature of the material is raised during the conditioning phase in order to promote plastic flow. Friction welding is a challenging process to model. There are extremely large temperature gradients in the vicinity of the weld interface and the material undergoes large deformations. Further challenges arise from the short and violent process to complete a weld, as well as the difficulties in obtaining experimental data throughout the process to complement, validate and inform the modelling effort. The objectives of this work are to model the macroscale multiphysical process leading to an accurate prediction of key process output variables, ultimately leading to a reliable method for predicting the post weld microstructure.

In order to model IFW, it is necessary to employ finite strain thermoelastoplasticity theory to capture the large, highly-coupled, plastic deformations observed during the process. To this end, a modified Johnson-Cook model capable of characterising both dynamic recrystallisation and strain rate softening in a phenomenological manner is employed. A crucial area of interest is the contact conditions, particularly at the weld interface, as this can have a significant effect on the simulated weld. The importance of this is further emphasised as there is little understanding of frictional contact mechanisms in IFW, including the transfer of material between the workpieces. The macro model will then allow for correct boundary conditions to be imposed on a meso model, capable of predicting the evolution of the principal phases of the nickel superalloy. These boundary conditions, such as the temperature history at a material point, can be extracted from the macro model by a “particle-tracking” algorithm allowing for simulation with thermodynamic modelling.

To mitigate the deleterious impact that the large deformations have on the quality of the Lagrangian discretisation of the domain, an automated remeshing scheme is implemented and the quality of the solution is monitored.

A series of numerical experiments elucidating the IFW process and demonstrating the robustness of the remeshing algorithm will be presented. The foundations for future work into the evolution of microstructure will also be shown.

Thermo-mechanical analysis of a steam turbine rotor

Johanna Eisenträger (*Otto von Guericke University, Germany*)

08:50

Konstantin Naumenko (*Otto von Guericke University, Germany*)

Yevgen Kostenko (*Siemens AG, Germany*)

Holm Altenbach (*Otto von Guericke University, Germany*)

In power plants, high temperatures prevail during long holding times. Furthermore, power plants are often started and shut-down in order to account for gaps or oversupplies in energy

production. These loading conditions induce both creep and fatigue loads. Due to their excellent thermo-mechanical properties, such as high tensile strength and elevated corrosion resistance, heat-resistant steels are established materials for power plant components. Nevertheless, these steels tend to soften under deformation, which should be accounted for by a constitutive model. The contribution at hand analyses the thermo-mechanical behavior of a steam turbine rotor. For this purpose, a unified phase mixture model is introduced. This constitutive model accounts for rate-dependent inelasticity, hardening, as well as softening by employing an iso-strain approach with a soft and a hard constituent. While the soft constituent represents areas with a low dislocation density, such as the interior of subgrains, the hard constituent refers to regions with a high dislocation density, i.e. the subgrain boundaries. Furthermore, two internal variables are introduced: a backstress tensor of Armstrong-Frederick type and a scalar softening variable. The model results in a coupled system of three evolution equations with respect to the inelastic strain, the backstress, and the softening variable.

To allow for the analysis of real power plant components, the model is implemented into the finite element method such that the evolution equations are integrated based on the backward Euler method. The applicability of the model is demonstrated by conducting a thermo-mechanical analysis of a steam turbine rotor with complex geometry under realistic boundary conditions. In a first step, the instationary temperature field in the rotor is computed in a heat transfer analysis. Thereby, typical steam temperatures in power plants and the corresponding heat transfer coefficients are prescribed. As a next step, the structural analysis is conducted based on the phase mixture model and the obtained temperature field as input. In addition, the time-dependent rotational frequency and steam pressure are taken into account. Note that the influence of different start-up procedures such as a cold or a hot start is examined in detail. As a result, the structural analysis provides the stress-strain hystereses, which constitute the basis for further fatigue and damage assessment.

Effect of crystallographic orientation in modelling of anisotropic plasticity with an analytical yield function

Selina Neuhaus (*Saarland University, Germany*)

09:10

Kinshuk Srivastava (*AG der Dillinger Hüttenwerke, Germany*)

Sebastian Scholl (*AG der Dillinger Hüttenwerke, Germany*)

Stefan Diebels (*Saarland University, Germany*)

The mechanical properties of dual- and complex-phase steels highly depend on their microstructure, which is formed during the production processes of the metal sheet. Additionally, an elastic-plastic anisotropy is encountered in these materials due to the distribution of the crystallographic orientations in the polycrystalline aggregate. The aim of the present work is to include plastic anisotropy in an already existing microstructure based model for the elasto-plastic deformation of dual-phase steels and thereby to widen the scope of such a model to a broader range of materials. The anisotropic plastic behavior can be described by two main approaches, namely choosing an appropriate phenomenological yield function or a polycrystal plasticity model.

The following contribution discusses the results of simulations on single- and bi-crystals by using different yield functions in order to accomplish a deeper understanding of the behavior and applicability of an analytical, anisotropic yield function in describing anisotropically deforming metals.

Numerical analysis of residual stresses on microscale and mesoscale in hot bulk forming parts under specific cooling

Sonja Uebing (*Universität Duisburg-Essen, Germany*)

09:30

Dominik Brands (*Universität Duisburg-Essen, Germany*)

Lisa Scheunemann (*Universität Duisburg-Essen, Germany*)

Mohammad Sarhil (*Universität Duisburg-Essen, Germany*)

Rainer Niekamp (*Universität Duisburg-Essen, Germany*)

Christoph Kock (*Leibniz Universität Hannover, Germany*)

Alexander Chugreev (*Leibniz Universität Hannover, Germany*)

Bernd-Arno Behrens (*Leibniz Universität Hannover, Germany*)

Jörg Schröder (*Universität Duisburg-Essen, Germany*)

Until now, the influence of residual stresses in metallic components is considered to reduce the durability and manufacturability, so that the potential of targeted residual stress states is still underachieved. Especially, in the course of its enhancement, hot forming processes can be useful since a number of parameters such as deformation state, temperature profile or cooling media can be adjusted independently. This contribution presents first steps towards a specific use of residual stress states in hot bulk forming parts.

For the simulation of residual stresses, a suitable material characterization and an appropriate numerical model are inevitable and require a good understanding of the thermal, mechanical and metallurgical properties of the material. Here, a multiscale view is considered to obtain a detailed description of the occurring characteristics, which is furthermore motivated by the classification of residual stresses in first, second and third type, acting on different scales. Therefore, upsetting tests of cylindrical specimen at high temperatures with specific cooling will be considered taking into account the microstructure. Numerical simulations using Finite Element Method (FEM), see [1], will be performed on the macroscale. Based on the results, microscopic simulations will describe the thermally-induced transformations on the microscale. The phase-field theory, see [2], as well as the FEM, see [3] will be utilized.

In this contribution, first results of the microscale simulations based on experimental and numerical data of the macroscale will be presented.

References

[1] B.-A. Behrens and P. Olle. Consideration of transformation-induced stresses in the simulation of press hardening. *Proceeding of International Plasticity*, 2008.

[2] I. Steinbach. Phase-field models in materials science. *Modelling and Simulation in Materials Science and Engineering*, 17(7):073001, 2009.

[3] D. Brands, D. Balzani, L. Scheunemann, J. Schröder, H. Richter and D. Raabe. Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from EBSD data. *Archive of Applied Mechanics*, 86:575-598, 2016.

On predictive modelling of yield stress increase in fresh cement paste

Haiqin Huang (*University of Luxembourg, Luxembourg*)

09:50

Andreas Zilian (*University of Luxembourg, Luxembourg*)

Freshly mixed concrete is composed of cement paste as fluid-like component and aggregates as solid particulate component. Development of yield stress in fresh mortar is significant for reliable and high-quality concrete operation as too low or too high yield stress causes processability challenges like the multilayer problem, aggregate floatation or blockage. Traditional experimental tests on the evolution of yield stress are costly since a wide spectrum of different material and environmental conditions needs to be studied. Progressing hydration, thermal effects and

mechanical loading/unloading may influence spatial distribution of the apparent yield stress. However, this local information is very difficult to obtain using traditional laboratory tests and virtual fresh concrete testing is therefore promising.

In the context of a multi-component flow approach to homogenised modelling of the mortar/aggregate composition at the macro-scale, the microstructural evolution affecting the development and distribution of apparent yield stress is taken into account by a thermo-chemo-mechanical phase-field model bridging the micro-macro length scales by using a Ginzburg-Landau-type free energy function. The phase-field, that describes the smooth spatial transition between fluid-like and solid-like behaviour of cement paste in the setting phase, is governed by bond-building chemical processes (hydration) and reversely-acting mechanical effects (bond breakup). The resulting set of coupled nonlinear advection-reaction-diffusion equations are formulated in the Eulerian framework and discretized in space using the weighted residuals method and finite differences in time. Implementation of the predictive model is demonstrated using the FEniCS framework, together with numerical examples supporting model validation.

Mixed XFEM formulation for the simulation of heterogeneities including elasto-plastic material behaviour

Stefan Löhnert (*Technical University of Dresden, Germany*)

10:10

The simulation of heterogeneous microstructures with significantly different material properties and stiffnesses often leads to locking effects if standard finite element approaches are employed, especially if the material behaves elasto-plastic according to von Mises plasticity. The eXtended Finite Element Method (XFEM) can be used to simulate arbitrarily shaped heterogeneities without meshing difficulties [1]. However, lower order XFEM elements also exhibit locking effects similar to standard finite elements.

In this contribution a mixed eXtended Finite Element approach for the simulation of heterogeneities is presented that leads to a locking free behaviour also for von Mises elasto-plastic behaviour and significantly different stiffnesses between the matrix and the inclusion material. The XFEM formulation is based on mixed Q1P0 formulation including enrichments for the displacement field as well as for the volumetric stress field [2]. On the element level static condensation can be applied, such that compared to the standard XFEM no additional degrees of freedom are necessary. The properties of the mixed XFEM formulation are compared to standard XFEM approaches by means of numerical examples and convergence studies.

References:

[1] N. Moes, M. Cloirec, P. Cartraud and J.-F. Remacle: A computational approach to handle complex microstructure geometries. *Comput. Methods Appl. Mech. Engrg.* 192 (2003) 3163 - 3177

[2] G. Legrain, N. Moes and A. Huerta: Stability of incompressible formulations enriched with X-FEM. *Comput. Methods Appl. Mech. Engrg.* 197 (2008) 1835 - 1849

S06.10 | Material modelling in solid mechanics

Date: February 21, 2019

14:00-16:00

Room: BIG HS

Application of model order reduction to a finite element model of cryogenic turning

Steven Becker (*Technische Universität Kaiserslautern, Germany*)

14:00

Hendrik Hotz (*Technische Universität Kaiserslautern, Germany*)

Benjamin Kirsch (*Technische Universität Kaiserslautern, Germany*)

Jan C. Aurich (*Technische Universität Kaiserslautern, Germany*)

Ralf Müller (*Technische Universität Kaiserslautern, Germany*)

In this talk, model order reduction is applied to a three-dimensional transient heat transfer problem of a workpiece during cryogenic turning [1]. Proper Orthogonal Decomposition (POD) is used to find an optimal projection base from a set of pre-computed solutions of the full-order model, that is to be projected onto a lower-dimensional subspace. In order to take advantage of the reduced system, the non-linear loading term, that arises by moving boundary heat fluxes, is hyper-reduced utilizing the Discrete Empirical Interpolation Method [2]. The reduced matrices are projected and accumulated on element level and the reduced global system of equations is solved by FEAP. The goal of the reduced model is to speed up the solution process of an inverse heat transfer problem, where the magnitude of boundary conditions is sought for a given set of temperature measurements.

References:

[1] S. Becker, H. Hotz, B. Kirsch, J. C. Aurich, E. von Harbou, R. Müller (2018): A Finite Element Approach to Calculate Temperatures Arising During Cryogenic Turning of Metastable Austenitic Steel AISI 347. In: J. Manuf. Sci. Eng. 140 (10), pp. 101016/1-101016/7.

[2] S. Chaturantabut, D. C. Sorensen (2010): Nonlinear Model Reduction via Discrete Empirical Interpolation. In: SIAM J. Sci. Comput. 32 (5), pp. 2737-2764.

On matrix representations of tensor algebra in continuum physics

Rainer Schlebusch (*Technische Universität Dresden, Germany*)

14:20

Nowadays, a computer often accomplishes the numerical solution of engineering continuum physics' problems by using the finite element method. The implementation of corresponding highly sophisticated constitutive models (such as anisotropic elasticity, viscoplasticity, piezoelectricity, etc.) into a computer software necessitates the conversion of abstract higher-order tensors into real numbers that can be processed by a computer. This quantification of tensors by real numbers is accomplished (1) by introducing bases and dual bases, and (2) by arranging the scalar tensor components into matrices. In literature, several such conversion processes can be found. Two of them are well known under the names of Voigt notation and Kelvin notation.

The best choice of that conversion process preserves the algebraic structure of a considered tensor equation. That is, (1) the scalar tensor components obtained during the conversion process for a tensor needs to be arranged in a special way into an associated matrix, and (2) the algebraic operations and mappings (such as duality pairings, dyadic products, inner products, linear mappings, invariants, eigenvalues, eigenvectors, etc.) in the considered tensor equation should be preserved by the corresponding matrix representations. Furthermore, the conversion process should use existing constraints (such as minor and major symmetries, linearized incompressibility, etc.) that might apply to the tensors to increase the numerical efficiency. Every redundant

information (for example equal scalar tensor components) should be removed from the matrix representation. Thus, in these special and very common cases in continuum physics, the effective size of the matrices are significantly reduced. Of course, the inverse conversion process should be available as well. As a result, the matrix representation of a tensor equation allows exploiting computational linear algebra libraries, and, hence, makes possible a numerically efficient processing of the tensor equation.

In this contribution, a universal conversion process for the matrix representation of a tensor equation will be presented, and conversion processes from literature will serve as examples.

Automatic generation of material laws based on rheological models using a genetic algorithm

Hans Wulf (*Technische Universität Chemnitz, Germany*) 14:40

Richard Gypstuhl (*Technische Universität Chemnitz, Germany*)

Robert Kießling (*Technische Universität Chemnitz, Germany*)

Jörn Ihlemann (*Technische Universität Chemnitz, Germany*)

Using rheological models is a standard method for formulating materials laws. The basic elements are elasticity, viscosity and plasticity, which are connected by parallel and serial connections. If unrestricted nesting of these connections is allowed, an infinite number of possible models arises. Each model can be represented by a tree structure. For one-dimensional models with linear basic elements, the corresponding material law can be constructed automatically from its tree structure. Hence, a large variety of material models can be constructed and tested by a suitable computer program. Of course, finding the model that provides the best match for some experimental data is desirable. Therefore, each model is fitted to the target experimental data using standard optimization methods. This is embedded into a program that searches for the model with the best fit. Here, a genetic algorithm is employed, which is specifically designed to search the space of models. The design of this algorithm is shown as well as the application to different examples.

Symmetries for 4th and higher order tensors in generalized continua

Marco Valerio d'Agostino (*INSA Lyon, France*) 15:00

Robert J. Martin (*Universität Duisburg-Essen, Germany*)

Alexandre Danescu (*Ecole Centrale de Lyon, France*)

Patrizio Neff (*Universität Duisburg-Essen, Germany*)

The classification of all fourth order anisotropic tensor classes for classical linear elasticity is well known. We review the mathematical procedure of how to obtain that. Then, we extend this classification to fourth order elasticity tensors acting on non-symmetric matrices and higher order tensors. These tensors naturally appear in generalised continuum models. Based on tensor-symmetrization we provide the most general form of these tensors for the case of orthotropic, transversely isotropic, cubic and isotropic materials. We give a self-contained presentation and at the end provide a detailed calculation for simple examples.

On the change of the reference configuration and its application within FEM simulation

Ralf Landgraf (*Chemnitz University of Technology, Germany*) 15:20

Jörn Ihlemann (*Chemnitz University of Technology, Germany*)

In solid mechanics, the initial state of a numerical simulation plays an important role and thus has to be defined properly. For example in inelastic material models (viscoelastic, plastic, etc.) the

current stress state is not only defined by the current loading state but also by the loading history. The consideration of the loading history is of special interest within simulations of multi-stage forming processes, where a change of simulation models between the different forming steps has to be applied. Here, an adequate transformation of the loading history between the simulation models has to be carried out to capture previous simulation steps. Another example is the analysis of thermo-mechanical processes including heat expansion. Typically, the coefficient of heat expansion is defined with respect to a fixed reference temperature. However, if a stress free specimen with a given geometry and a certain initial temperature unequal to the reference temperature is modelled, then an unrealistic volume change of the specimen would occur within the first calculation step. Similar phenomena would occur, if further volume changing processes (e.g. curing shrinkage) are regarded.

In this contribution, the above described examples and the corresponding change of the reference configuration are addressed. Proper transformation rules as well as their implementation into commercial finite element codes are provided. The considered material models include a model of multiplicative viscoplasticity for the simulation of multi-stage forming processes as well as a general model for the simulation of curing phenomena (including heat expansion and chemical shrinkage). Finite element simulation examples with and without adequate consideration of changing reference configurations will highlight the necessity of employing adequate transformation rules.

A juxtaposition of data driven and stochastic finite element analyses for problems with noisy material data

Tim Fabian Korzeniowski (*Universität Siegen, Germany*)

15:40

Thomas Reppel (*Universität Siegen, Germany*)

Kerstin Weinberg (*Universität Siegen, Germany*)

In the data driven finite element analysis the constitutive material modeling is elided and instead experimental data are directly employed as an input for computational analysis. Our contribution focuses on a comparison of this approach to more traditional finite element methods. The point of departure is a given set of noisy material data which requires simplification and / or uncertainty modeling of the material. We illustrate the methodology of data driven solutions, stochastic finite element solutions and analytic solutions under such material uncertainties. Numerical examples are used to show the pros and cons of the given methods. Furthermore we explore the usage of the data driven modeling within different applications and also take a look on the acquisition of the multi-dimensional data fields needed.

S06.11 | Material modelling in solid mechanics

Date: February 21, 2019

14:00-16:00

Room: SR 05

Modelling of cellular materials by a microsphere-based material model

Anne Jung (*Saarland University, Germany*)

14:00

Thomas Bleistein (*Saarland University, Germany*)

Stefan Diebels (*Saarland University, Germany*)

Metal foams are biomimetic cellular materials that mimic the structural elements of bones and wood. Based on their complex porous microstructure, the global mechanical properties depend strongly on the geometry and material properties of the individual struts. Pure continuum mechanical phenomenological models guarantee the modelling of large-sized problems with less

computational effort, but require extensive experimental studies for a reliable identification of the model parameters. The conclusive not only uniaxial but also multiaxial macroscopic characterization of foams is very complex, time-consuming and must be repeated with each change of the microstructure. Micro models take the cellular morphology directly into account by using real microstructures to achieve a realistic deformation mechanism. Such heterogeneous models, however, consist of an immense number of degrees of freedom leading to huge equation systems that make micro models computationally expensive.

The present contribution focuses on the development of a phenomenological macro model enriched with microstructural information. Therefore, a microsphere-based model is used, which establishes a reference to the micro level of individual struts. The idea of microsphere models is to describe the global 3D mechanical behavior of a component by 1D material models applied to different directions in a unit sphere, where each Gauss point of a finite element is described by such a unit sphere. Experimental micro tensile tests and micro compression tests on individual struts of open-cell aluminum foams were used to describe the unknown 1D material model by a piecewise interpolated elastic 1D constitutive material law. Since different 1D constitutive laws are required to describe the material response of the micro tensile tests and micro compression tests respectively, the global microsphere model in its 3D generalization directly accounts for anisotropies in the material behavior under tensile and compression loading.

Static wetting on stretched soft substrates

Stefanie Heyden (*ETH Zurich, Switzerland*)

14:20

Robert Style (*ETH Zurich, Switzerland*)

Katrina Anne Smith-Mannschott (*ETH Zurich, Switzerland*)

Eric Dufresne (*ETH Zurich, Switzerland*)

Young's law for wetting on rigid substrates and Neumann's triangle for wetting on liquid substrates represent two well-known solutions, which are at the same time two extreme cases of wetting problems (i.e., infinitely hard versus infinitely soft substrates). Recently, solutions accessing the spectrum of intermediate behavior have been presented for droplets of arbitrary radius on thin solid substrates. Results show that for large droplets, Young's law is recovered for the macroscopic contact angle, whereas a lenticular shape as predicted by Neumann's analysis constitutes the macroscopic behavior for small droplets. The microscopic behavior close to the contact line however is governed by Neumann's triangle for droplets of all sizes. Here, we extend solutions for droplets of arbitrary radius on thin solid substrates to also account for pre-stretched substrates as utilized in experiments. Stretched substrates thereby allow us to break symmetry and hence access more information on the intermediate deformation regime.

Soil modelling with a DEM-Lookup approach

Jonathan Jahnke (*Fraunhofer ITWM, Germany, Technische Universität Kaiserslautern, Germany*)

14:40

Stefan Steidel (*Fraunhofer ITWM, Germany*)

Michael Burger (*Fraunhofer ITWM, Germany*)

We consider the interaction of digging tools with soil using a two phase lookup approach. The modelling of soil to predict draft forces is a difficult endeavor. The most wide-spread approach is the discrete element method. While numerics are relatively simple relying mostly upon explicit ODE-solvers, the correct parametrization of the model is challenging. We present a fast and reliable DEM-method which relies upon a scale-independent contact law. The problem of simulation speed is addressed when it comes to real-time applications. A lookup table approach based on an offline simulation phase and an online lookup phase is presented. We show the validity of our approach with measurements using relevant laboratory experiments and comparing them to simulations.

An extended hypoplastic model incorporating the coordination number for the simulation of granular flow

Abdiel Ramon Leon Bal (*Ruhr University Bochum, Germany*)

15:00

Thai Son Dang (*Ruhr University Bochum, Germany*)

Günther Meschke (*Ruhr University Bochum, Germany*)

A computational excavation model for soft soils in water-saturated conditions is presented. The proposed method couples a Particle Finite Element (PFEM) re-meshing strategy with an extended hypoplastic model based on a model proposed by Guo et.al, where the total stress is decomposed into a quasi-static part described by a hypoplastic model and a strain rate-dependent dynamic part. The viscoplastic extension of the constitutive model is based on the theory of dispersive pressure in concentrated granular suspensions proposed by Bagnold. Grain collisions and interstitial fluid viscosity are identified as the two primary mechanisms for the rate effects in the granular medium. The dominance of each contribution defines two distinct flow regimes related to grain inertia and viscous effects, which are established by means of the Bagnold number. Relevant state and material parameters of the extended formulation include the diameter of solid particles, the linear grain concentration, the interstitial fluid viscosity and the normal to shear stress ratio.

In this work, we propose an enhancement of the extended model by incorporating information of the grain interaction through the coordination number, which is the average number of grain-to-grain contacts per particle. The spatio-temporal evolution of the coordination number comes as a reliable indicator of the shear and dilatancy behavior experienced by granular soils and on its solid-fluid transition mechanism. We propose the modification of the dynamic component of the model by considering directly the coordination number and its critical value as state parameters. Discrete Element Method (DEM) simulations are employed as the numerical tool to support the computational experiments for the determination of the coordination number of the particles, its evolution and correlation to the parameters pertaining to the grain assembly.

Selected numerical benchmarks will be presented for the validation of the model, characterized by soft soil excavation experiments. Computational simulations of rigid cutting tools excavating soft soils under fully saturated conditions are performed to demonstrate the performance of the proposed formulation.

On the structural correlation in plastically deformed disordered materials

Franz Bamer (*RWTH Aachen University, Germany*)

15:20

Jan Stratmann (*RWTH Aachen University, Germany*)

Firaz Ebrahim (*RWTH Aachen University, Germany*)

Bernd Markert (*RWTH Aachen University, Germany*)

We investigate the mechanical properties of non-crystalline materials on the nanoscale. Using molecular dynamics, we analyze ductile behavior of silica glass [1] and link its plastic deformation with the network topology [2]. The objective of the present contribution is to further understand the plastic mechanism in disordered materials with particular emphasis on the network structure. Therefore, we introduce lately discovered two-dimensional materials, e.g. [3], which enable to visually track atomic rearrangements. The samples are subjected to tensile and shear deformation. In order to eliminate both temperature effects as well as deformation rate dependence, an athermal quasistatic deformation scheme is applied [4] using a step-by-step loading minimization procedure.

[1] F. Ebrahim, F. Bamer, B. Markert, *Comput. Mater. Sci.* 149 (2018) 162-169.

[2] F. Bamer, F. Ebrahim, B. Markert (in press), *J. of Non-Crystal. Solids*, <https://doi.org/10.1016/j.jnoncrysol.2018.09.043>.

[3] P.Y. Huang et al., *Nano Lett.* 12 (2012) 1081-1086.

[4] D. Rodney, A. Tanguy, D. Vandembroucq, *Model. Simul. Mater. Sci. Eng.* 19 (2011) 083001.

S06.12 | Material modelling in solid mechanics

Date: February 21, 2019

17:40-18:40

Room: BIG HS

Modeling deformation-dependent interface energies by means of phase-field theory

Henning Lammen (*TU Dortmund, Germany*)

17:40

Jörn Mosler (*TU Dortmund, Germany*)

Within classic phase field theories of Allen-Cahn- or Cahn-Hilliard-type, phase transformations are governed by a competition between bulk and interface/surface energies. For deformation-driven phase transformations, such energies might depend on the phase field parameter as well as on the deformation. However, the latter dependency is usually not considered as far as the interface is concerned. While this assumption can be reasonable for some specific applications, it eliminates the interesting and important size effect due to mechanical loading. For instance, as shown in [1,2], a deformation-dependent sharp interface embedded in a bulk matrix can result in a classic “the smaller the stronger” relation, but also in the inverse “the smaller the softer” relation. Depending on the deformation-dependent energetics of the interface, even non-monotonous size effects can be observed. Within the present talk, deformation-dependent interface/surface energies are approximated by means of phase field theory. It is shown that the results as reported in [1,2] can be consistently approximated.

[1] T. Heitbreder, N.S. Ottosen, M. Ristinmaa, J. Mosler. On damage modeling of material interfaces: Numerical implementation and computational homogenization. In: *Computer Methods in Applied Mechanics and Engineering* 337 (2018), 1-27, <https://doi.org/10.1016/j.cma.2018.03.023>.

[2] A. Javili, P. Steinmann, J. Mosler. Micro-to-macro transition accounting for general imperfect interfaces. In: *Computer Methods in Applied Mechanics and Engineering* 317 (2017), 274-317, <https://doi.org/10.1016/j.cma.2016.12.025>.

On higher-order interface models

Tim Heitbreder (*TU Dortmund University, Germany*)

18:00

Jörn Mosler (*TU Dortmund University, Germany*)

Interface models are well established and frequently applied in material science. Classical non-coherent interface models such as cohesive zone models are described by a Helmholtz energy depending on the displacement jump. The extension to thermodynamical consistent combination of classical non-coherent cohesive zone models with surface elasticity is still relatively new, cf. [1] and [2]. These models depend on the displacement jump as well as on the surface deformation gradient. In this talk, the impact of higher-order gradients will be investigated. It will be shown, that the gradient of the displacement jump does not lead to new findings on the material behavior. By way of contrast, the gradient of the surface deformation gradient, captures curvature effects of an interface. Representative examples will demonstrate this.

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[2] T. Heitbreder, N. S. Ottosen, M. Ristinmaa and J. Mosler, “On damage modeling of material interfaces: Numerical implementation and computational homogenization”, *CMAME*, 337, 1-27, (2018).

Effect of surface energy anisotropy on diffusion controlled process in polycrystalline materials

Asim ullah Khan (*Ruhr-Universität Bochum (RUB), Germany*)

18:20

Klaus Hackl (*Ruhr-Universität Bochum (RUB), Germany*)

Matthias Baitsch (*Ruhr-Universität Bochum (RUB), Germany*)

The objective of this work is to study the effect of anisotropic surface energy on morphological evolution in polycrystalline materials. When grain boundary comes in contact with the free surface in polycrystalline materials, there are formations of grooves. Diffusion is a dominant phenomenon for these formations below the roughening temperature. We use a finite element model for thermal grooving, already presented by Hackl et al. This model includes diffusion along free surfaces and along the triple lines [1]. The surface energy of each grain is calculated using an orientation dependent energy model in three dimensions. In certain grain orientations, groove profiles are different from Mullins classical theory. These formations have planar faces with no measurable curvature. It is due to high anisotropy in surface energy. With an increasing anisotropy, we have accelerated pit formation at quadruple points. The growth rate of triple lines and quadruple points follows $1/4$ power law. This model gives converging results even in the critical range of anisotropy. Grain boundary and triple line energies are assumed isotropic and constant. Comparative studies show the effect of varying mobilities on growth kinetics and groove shapes.

S06.13 | Material modelling in solid mechanics

Date: February 21, 2019
Room: SR 05

17:40-18:40

Modeling the curing process of a polyurethane structural adhesive with regard to the mechanical properties of the cured material

Rebecca Jennrich (*Bundeswehr University Munich, Germany*)

17:40

Alexander Lion (*Bundeswehr University Munich, Germany*)

Michael Johlitz (*Bundeswehr University Munich, Germany*)

Sarah Ernst (*Technische Universität Braunschweig, Germany*)

Elisabeth Stammen (*Technische Universität Braunschweig, Germany*)

In the context of lightweight construction and modern hybrid technologies, the importance of structural and soft adhesives in the automotive industry is increasing. Polyurethane adhesives are relatively soft, show nonlinear viscoelastic behavior at room temperature and can endure large deformations. Therefore, they are well suited for applications under dynamic loadings and can compensate gap changes generated by materials with different thermal expansion coefficients. Theoretically, the examined adhesive can be cured either thermally or through humidity, resulting in the same mechanical characteristics. In order to minimize the process time in industrial applications the curing temperature must be increased without negatively affecting the mechanical properties of the bond. To this end, the metallic joint partner can be induction heated resulting in high heating rates of about 100 to 150 K/min on the adhesive's surface. In comparison with metals polyurethane conducts the heat with a much smaller rate which results in higher temperature gradients within the adhesive layer. The goal of this project is the modeling of a fast-curing polyurethane adhesive under consideration of the changes in the density and the thermomechanical material properties induced by curing, followed by the identification of material parameters to ultimately optimize the curing process.

On the singular integro-differential equations related to the adhesive interaction of elastic patch and plate

Otar Jokhadze (*Tbilisi State University, Georgia*)

18:00

Nugzar Shavlakadze (*Tbilisi State University, Georgia*)

The problem of constructing an exact or approximate solutions of system of singular integro-differential equations related to the problems of adhesive interaction between elastic thin finite or infinite nonhomogeneous patch and elastic plate is investigated. For the patch loaded with horizontal and vertical forces the usual model of beam bending in combination with the uniaxial stress state model is valid. Using the methods of theory of analytic functions, integral transformation or orthogonal polynomials the singular integro-differential equations reduced to the different boundary value problems (Karleman type problem with displacements, Riemann problem) of the theory of analytic functions or to the infinite system of linear algebraic equations. The asymptotic analysis of problem is carried out.

Material modelling of hyperelastic silicone adhesives considering stiffness reduction

Elisabeth Toups (*RWTH Aachen University, Germany*)

18:20

Stefanie Reese (*RWTH Aachen University, Germany*)

Jaan-Willem Simon (*RWTH Aachen University, Germany*)

Load bearing bonds become increasingly common in glass-façade structures due to their beneficial characteristics, such as the more continuous load transfer between glass and the supporting elements compared to alternative connections, and the possibility to enable a more transparent design [1], [2]. The used adhesives exhibit a hyperelastic material response and behave as a rubberlike material under large deformations. Furthermore, stiffness reduction is observed during experimental investigations, as described by the Mullins Effect.

Current German regulations of dimensioning such load bearing bonds include very high safety factors [3] which could be reduced by a better prediction of the real material behaviour [4]. To provide better predictions, a material model representing all the mentioned properties is needed to enable a less time consuming and less cost intensive realistic calculation and dimensioning.

From literature material models are available, but most of them are not able to simulate the described material behaviour, namely large deformations combined with stiffness reduction and multiaxial stress states. For this reason a new model is developed, which is based on the Ogden formulation for hyperelastic materials combined with a continuum damage approach. Taking into account stiffness reduction during loading and unloading procedures a new variable is defined and considered specifically in each Ogden term. For the ideal calibration of the material parameters different experiments such as simple tension, pure shear and equibiaxial tension are considered during the fitting procedure. For validation, several examples, taking into account multiaxial stress states, are analysed and discussed.

References

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S06.14 | Material modelling in solid mechanics

Date: February 22, 2019

08:30-10:30

Room: BIG HS

Experimental investigation of material parameters from direct laser writing

Wenjie Huang (*TU Kaiserslautern, Germany*)

08:30

Our micro robots are of great interest for medical applications because they can transport and release drugs in human body or interact with diseased tissue without surgery. The dimensions of our robot range from a few to hundreds of micrometers. To produce them, we are using direct laser writing. Our goal is to create a mussel-shaped robot that can open and close its shells by an externally applied magnetic field. For direct laser writing, different printable materials are available. We mainly use two of them: the standard photoresists (IP-S from Nanoscribe GmbH) and the liquid crystal elastomers (from Synthon Chemicals).

This work presents investigations of Young's modulus and thermal expansion coefficients of laser-written samples. The material properties are directly related to the process parameters of direct laser writing, such as laser intensity, writing speed and line spacing. The knowledge of the dependencies between the process parameters and the material properties is the first step for the later design and production of our micro robots.

Samples with different writing parameters were prepared for the tests. However, these samples are so small that conventional tensile tests are not suitable for measuring their elastic properties. Instead, we are using a nanoindentation test. In addition, we have designed a test setup for the investigation of thermal expansion in which the small test specimens can be heated and observed with a CCD camera. Images of samples at different temperatures have been taken so that their thermal expansion can be investigated and their coefficients of thermal expansion determined by image processing.

The results are useable for producing our micro robots with specially adapted material properties. Especially for the control and operation of the robots, material property dependent mechanisms open up new possibilities.

Identification of parameters using iterative bipolar target functions

Niklas Nostitz (*Deutsches Institut für Kautschuktechnologie e.V., Germany, Chemnitz University of Technology, Germany*)

08:50

Nils Hendrik Kröger (*Deutsches Institut für Kautschuktechnologie e.V., Germany*)

Jörn Ihlemann (*Chemnitz University of Technology, Germany*)

The identification of material parameters is a required process for industrial applications to characterize the used material models. While standard procedures to identify these parameters are often established via methods based on the Gauss-Newton algorithm, improvements are still possible.

One problem is the simultaneous identification for multiple data sets. These different experimental sets represent technical applications of the component. Further, an optimization with respect to a L2-error function is not always the optimal objective. More important is the simulation curve's shape and its position in a certain corridor. Such a corridor for optimal curves can

have multiple reasons like side conditions based on theoretical identifications via FEM, statistical deviations in the production process or prescribed values.

The control of this corridor is not possible by a simple weighting. Because of these requirements a new error function has to be defined. Additionally, the new error function should be C2-continuous at the corridor borders. To fulfill these conditions, the new error function is built via different parabolic function parts and is named “biparabolic target function”. The choice of the corridor can depend on the data lying within: a single loading curve, a cycle or even different curves. Beside this new formulation an iterative change of the border curves defining the corridor is possible as well. This leads to an identification, where the quality of the enclosed data points can be increased and the corridor depended material parameters can be examined.

In order to test this new method, we look into an experimental data set originating from different homogenous specimens. The error function of one experiment is related to a corridor. The overall behavior of the solutions is examined based on the choice of the border curves and the formulations of the biparabolic target functions. As a result, the biparabolic approach leaves more opportunities to choose a suitable solution.

In a second step an iterative correction of the corridor borders is applied. The consequences of this new iterative method are examined and compared to a simple weighting approach. The advantages of the new formulation can be shown.

Influence of thermal boundary conditions on the parameter identification in thermodynamics

Lars Rose (*TU Dortmund, Germany*)

09:10

Andreas Menzel (*TU Dortmund, Germany, Lund University, Sweden*)

The Finite Element (FE) based parameter identification is an already well tested method for the identification of material parameters of mechanical material models. Key part of such an identification is a FE-solution of a boundary value problem which shall represent the actual experimental conditions as closely as possible. This does not only include the geometry of the specimen but also the applied boundary conditions. The latter are usually intuitively known for the mechanical field. If a thermo-mechanically coupled material model is considered, however, thermal boundary conditions must also be defined. For most experiments, these thermal conditions are of the Robin type and require the temperature of the surrounding medium as well as a coefficient which describes the quality of heat exchange. Especially the so called convection coefficient is unknown in general so that an ansatz for the identification of these coefficients is presented. Furthermore, the influence on the result of a parameter identification for a thermo-mechanically coupled material model is discussed using full field measurements of the displacement field as well as of the temperature field.

Parameter identification of strain rate dependent hardening for sheet metals

Benjamin Söhngen (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

09:30

Kai Willner (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

Minimizing production costs and overall weight of products is a major goal for manufacturers in the 21st century. One way to address this aim is the simulation of complex forming processes by means of finite element method (FEM) for process and design optimization. For this purpose, an adequate material model has to be chosen and the corresponding parameters have to be identified.

In this contribution we examine the influence of strain rate on the isotropic hardening of two sheet metals. The nominal strain rates vary between 0.0005 1/s and 20 1/s and the full field

deformation is captured with the help of digital image correlation (DIC) technique. For modeling the strain rate dependent hardening behaviour, phenomenological laws like "Johnson-Cook" have become established. We distinguish between approaches that incorporate the rate dependency in an additive or multiplicative manner and identify which best describes the experimental measurements.

The hardening laws are thereby embedded in a large strain plasticity framework based on the logarithmic strain space as presented in [1] and [2] for the application with kinematic hardening resp. anisotropic plasticity. The material parameters are identified both in a direct fashion, where the gap between the constitutive equations and the measured stress-strain-curves is minimized and indirectly by using FEM to generate force-displacement-curves.

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Towards deep learned constitutive models based on two-dimensional strain fields

Markus Hillgärtner (*RWTH Aachen University, Germany*)

09:50

Kevin Linka (*RWTH Aachen University, Germany*)

Mikhail Itskov (*RWTH Aachen University, Germany*)

In order to calibrate material models, experimental stress-strain curves are usually compared with model predictions under the same loading conditions. While this approach guarantees good results for one specific loading type, the resulting model is not generally able to properly predict other loading scenarios. Therefore, a variety of mechanical tests can be conducted, amongst which uniaxial tension, uniaxial compression, pure-shear and equibiaxial tension tests are the most commonly used ones. Multi-axial loading often cannot be adequately predicted solely based on test data of one such idealized test. Therefore, the material model can be fitted against several mechanical test data sets simultaneously in order to increase the prediction quality, which requires a considerable amount of experiment work.

This contribution aims to create phenomenological material models which are directly fitted against an experimental force response and the corresponding two-dimensional strain field obtained from arbitrary loading. To this end, a deep learning framework based on a multilayer-perceptron (MLP) approach [1] is proposed which identifies suitable strain-energy functions and its corresponding derivatives. These can be utilized in a commercial finite element code via a user defined material subroutine in order to compare the quality of the approximation with the reference data. This approach skips idealized experiments and simplifies the process of phenomenological modeling by exploiting the capabilities of deep neural networks.

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S07 | Coupled problems

Organiser: Detlef Kuhl (*University of Kassel, Germany*)
Ralf Jänicke (*Chalmers University of Technology, Sweden*)

S07.01 | Coupled problems

Date: February 19, 2019
Room: HS 21

08:30-10:30

On the motion of a bubble-soap: the Navier-Stokes equations coupled with surface tension forces on an immersed interface

Sébastien Court (*University of Graz, Austria*)

08:30

We consider a two-phase flow governed by the incompressible Navier-Stokes equations. The domain is split into two connected parts by an immersed manifold of codimension 1. This manifold is an interface without thickness, and represents a bubble-soap that we see as a smooth perturbation of the sphere. On this interface, a surface tension force, proportional to the mean curvature of the manifold, induces a jump of the normal trace of the Cauchy stress tensor on both sides. The response of the fluid is the equality of velocities at this interface. The value of this velocity determines the time evolution of the interface, and this is how the dynamics of the bubble-soap is coupled with its own geometry. Questions relative to the existence of solutions and their asymptotic stability will be evoked. In particular, we describe the time evolution of the manifold with an abstract PDE whose operator formulation can be exploited for further control and stabilization problems. Simulations of such a model require special treatments. We address this issue by developing a mixed stabilized finite element method coupled with a fictitious domain approach.

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[2] S. Court. A fictitious domain approach for a mixed finite element method solving the two-phase Stokes problem with surface tension forces. arXiv:1807.09894

A concept for aortic dissection with fluid-structure-crack interaction

Richard Schussnig (*Graz University of Technology, Austria*)

08:50

Thomas-Peter Fries (*Graz University of Technology, Austria*)

Substantial advances in the computational modeling of the cardiovascular system and its pathologies were made during the last decades. Both, chronic and acute aortic dissection are highly dangerous health conditions, requiring medication, monitoring or immediate surgical treatment. It is expected that a proper modeling and simulation may significantly help to understand the sequence of events ultimately leading to the rupture of aortic layers forming a propagating false lumen and/or complete rupture of the aorta.

Aortic dissection may be interpreted as a fluid-structure interaction application where the blood flow and the tissue deformation are strongly coupled [1, 2]. A major challenge is that the rupture of aortic layers features a moving crack front which, being part of the fluid-structure interface, largely effects the flow field. The arterial wall is modeled as a hyperelastic solid governed by the geometrically nonlinear elastodynamics equations and the haemodynamics are represented

by the instationary Navier-Stokes equations for incompressible fluids in arbitrary Lagrangian-Eulerian form, following [3]. The crack path of the dissection is, at this stage, predefined, only the propagation of the crack tip along the path over time is part of the solution. A simple traction-separation law as in cohesive fracture is used in this study. Hence, the fluid domain is evolving in time. The strong coupling of the involved fields (i) structure mechanics, (ii) fluid mechanics, and (iii) crack propagation is crucial for simulating the rupture process in aortic dissection. Herein, a concept is outlined in two spatial dimensions, which is later extended to the three-dimensional case.

References

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- [2] Reymond, P.; Crosetto, P.; Deparis, S.; Quarteroni, A. and Stergiopoulos, N.: Physiological simulation of blood flow in the aorta: Comparison of hemodynamic indices as predicted by 3-D FSI, 3-D rigid wall and 1-D models. *Medical Engineering & Physics*, 2013, 35, 784-791
- [3] Küttler, U.; Gee, M.; Förster, C.; Comerford, A. and Wall, W.: Coupling strategies for biomedical fluid-structure interaction problems. *International Journal for Numerical Methods in Biomedical Engineering*, 2010, 26, 305-321

Solid-fluid coupling in a fully Lagrangian framework

Jens Bender (*Fraunhofer ITWM, Germany, University of Kaiserslautern, Germany*) 09:10
Jörg Kuhnert (*Fraunhofer ITWM, Germany*)

The simulation of multiphase flows including granular and fluid phases is of great interest in a wide variety of industrial applications, such as chemical process engineering, design of conveyor systems or abrasion modeling. In this context, the granular phase is often described by the discrete element method, which calculates the trajectory of each individual solid particle in a Lagrangian manner while resolving inter-particle and geometry collisions. While the models behind individual interactions are generally not very complex, the necessary data structures and neighborhood algorithms often have a major impact on performance. Here, we present the coupling of this approach to an existing Lagrangian generalized finite difference method for the fluid phase. It is developed at Fraunhofer ITWM and has been successfully used in a wide variety of practical applications. Coupling these two approaches enables us to treat all phases in a common framework and to use the existing efficient and scalable data structures and algorithms, while also benefiting from the advantages of meshfree fluid solvers in free surface problems or rapidly changing flow geometries.

A novel multi-vector interface quasi-Newton method for partitioned fluid-structure interaction

Thomas Spenke (*RWTH Aachen University, Germany*) 09:30
Norbert Hosters (*RWTH Aachen University, Germany*)
Marek Behr (*RWTH Aachen University, Germany*)

Partitioned solution schemes for fluid-structure interaction are widely used in modern computational engineering science, as they offer a great flexibility and modularity concerning the two solvers employed for the fluid and the structure. Their major downside, however, is an inherent instability caused by the so-called added-mass effect [1]. Depending on the application, its influence might be severe enough to impede a numerical solution - if no counter-measures are taken.

In recent years, interface quasi-Newton methods have gained growing attention in the fluid-structure interaction community by significantly improving partitioned solution schemes: They not only manage to seize control of the added-mass instability, but also prove to substantially speed up the coupling’s convergence. Identifying the converged solution as a fixed point of the boundary deformation, their basic idea is to accelerate the coupling iteration using Newton’s method. Since the required (inverse) Jacobian in general is not accessible, interface quasi-Newton approaches settle for approximating it instead [2].

In this work, we present a new interface quasi-Newton variant: The key idea is to seize on the multi-vector Jacobian update scheme first presented by Bogaers et al. [3], while avoiding any explicit representation of the (inverse) Jacobian approximation, since it slows down the solution for large systems. Instead, all terms involving a quadratic complexity have been systematically eliminated. The result is a new multi-vector interface quasi-Newton variant whose computational costs are scaling linearly with the problem size.

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Model order reduction of parameterised monolithic fluid-structure interaction

Daive Baroli (*University of Luxembourg, Luxembourg*)

09:50

Andreas Zilian (*University of Luxembourg, Luxembourg*)

Predictive numerical analysis of fluid-structure interaction is often prohibitively expensive if the state of complex systems is subject to parameter variations (e.g. structural/fluid material properties, kinematic/dynamic boundary conditions, Reynolds number). If the space of parameter variations is known, reduced-order solution methods can be established that consist of a computationally expensive offline stage evaluating a high-fidelity model of the coupled system and a fast online stage deploying a low-order representation of the same.

This contribution investigates different strategies for basis generation and online evaluation in a projection-based approach to reduced order modelling. For this, the starting point is a monolithic formulation of the boundary-coupled problem involving a deforming interface. The fluid is described with the incompressible Navier-Stokes equations in an Arbitrary Lagrangian-Eulerian (ALE) framework, pulled back to the reference configuration of the fluid domain and using velocity and pressure as unknowns. In order to facilitate native kinematic coupling at the fluid-structure interface, the solid is formulated in a mixed-hybrid velocity/stress approach using the rate form of a polyconvex complementary strain energy function. The velocity of the deforming fluid domain is simultaneously taken into account with a pseudo-structure approach and allows the evaluation of the resulting highly nonlinear ALE weak form in a truly monolithic fashion. Describing all involved fields on their fixed reference configuration simplifies the generation and use of reduced bases during the model reduction process.

The highly nonlinear monolithic model is implemented using the FEniCS framework. Nonlinearities will be particularly addressed by employing recent hyper-reduction approaches. The efficiency and quality of the resulting low-order models will be discussed for different parameterised FSI benchmark problems.

Numerical solution of viscoelastic fluid-structure-diffusion systems with applications in ophthalmology

Alexander Drobny (*Heidelberg University, Germany*)

10:10

Elfriede Friedmann (*Heidelberg University, Germany*)

The research of fluid-structure interaction problems is a continuously growing field, especially regarding applications in medicine and biology. We present the coupling of a potentially viscoelastic fluid with multiple hyperelastic structures incorporating chemical processes in the arbitrary Lagrangian Eulerian framework. This monolithic formulation allows a robust numerical solution with Newton's method. The discretization is based on the shifted Crank Nicholson scheme for temporal discretization and the Galerkin finite element method for spacial discretization. This fluid-structure interaction problem is applied to ophthalmology in order to improve the medical treatment of retinal diseases. The physiological processes include the elastic response of various structures like the sclera, lens and iris coupled to the fluid-like vitreous which is modelled by a viscoelastic Burgers type model for the healthy case and by the Newtonian Navier-Stokes equations for the pathological case. Since most medical treatments are based on the injection of medicine we furthermore study the drug distribution, which is modelled by the convection-diffusion equation, in the whole eye for healthy and non-healthy pathologies.

S07.02 | Coupled problems

Date: February 19, 2019

16:30-18:30

Room: HS 21

A least-squares finite element approach to model fluid-structure interaction problems

Solveigh Averweg (*University Duisburg/Essen, Germany*)

16:30

Alexander Schwarz (*University Duisburg/Essen, Germany*)

Carina Nisters (*University Duisburg/Essen, Germany*)

Jörg Schröder (*University Duisburg/Essen, Germany*)

In this contribution an approach to model fluid-structure interaction problems with monolithic coupling is presented. The fluid as well as the structural domain are discretized using the least-squares finite element method (LSFEM), whose application results in a minimization problem with symmetric positive definite equation systems also for non self-adjoint problems. In this study, the second-order systems are reduced to first-order systems by introducing new variables, which leads to least-squares formulations for both domains based on the stresses and velocities as presented in e.g. [1] and [2]. A conforming discretization of the unknown fields in H^1 and $H(\text{div})$ using Lagrange interpolation polynomials and vector-valued Raviart-Thomas interpolations functions leads to the automatic fulfillment of the coupling conditions. In more detail, a discretization in H^1 ensures continuity of the velocity field and a discretization in $H(\text{div})$ results in continuity of the normal stress components at the interface.

References

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Thermo-mechanical fluid-structure interaction of thermal buckling

Katharina Martin (*RWTH Aachen University, Germany*)
Stefanie Reese (*RWTH Aachen University, Germany*)

16:50

Experiments have shown that aerothermodynamical loads induced by high enthalpy flow on thin metallic panels in combination with unavoidable constraints for the movement of the structure might lead to undesirably localized plastic deformation and buckling phenomena. In the considered supersonic flow at Mach numbers of $Ma = 7.7$, the buckling of panels into the stream flow creates shocks and expansion areas which significantly impact the efficiency. In this work the fluid-structure interaction between the panel and the flow are shown.

An important part of the structural model is the description of the material behaviour. This requires a fully thermomechanical coupled viscoplastic model including large deformations. Therefore a realistic description of the highly temperature- and rate-dependent material behaviour of the structure must be considered. Besides convection and heat radiation, the temperature dependence of the mechanical material behavior as well as the deformation dependence in conduction and capacity terms have to be included in the thermomechanical coupling. For that an extended thermomechanical model is used which takes non-linear thermal evolution into account. This is achieved by defining a heat capacity which is nonlinearly dependent on the temperature. Therefore, a thermodynamically consistent model of finite thermo-viscoplasticity with non-linear kinematic hardening and isotropic hardening for large deformations is chosen. The Helmholtz energy includes nonlinear functions of the temperature and the isothermal energy, which decomposes into an elastic, a kinematic and an isotropic hardening part. To avoid locking effects, which occur for standard linear elements, and to reduce computational time, the material model is included in a solid-shell framework with reduced integration and hourglass stabilization.

For the fluid simulation the focus lies on studying the difference between a steady-state and a transient time integration. The flow composition of five species is also fully resolved and the effect in comparison to an ideal gas formulation will be shown.

A loose fluid-structure interaction is chosen, which provides the opportunity to couple two different commercial codes. The fluid-structure interaction focuses on the choice of an equilibrium iteration method, the time integration and the data transfer between grids.

Numerical and experimental research on effect of constraint methods on welding residual stress and nanomechanical performance of aluminum AA5083

Tianci Li (*Fraunhofer Insitut of Laser Technology, Germany, Beijing Jiaotong University, China*)

17:10

Lele Zhang (*Beijing Jiaotong University, China*)

Weiyuan Dou (*Beijing Jiaotong University, China*)

Xiaowei Wang (*DB International GmbH Beijing, China*)

AA 5083 welding structure is widely used in advanced engineering structures due to its lightweight and high strength weight ratio. In this study, the effects of two different constraint methods on the welding residual stress distribution, distortion and young's modulus in fusion zone and substrate were investigated. Welding residual stresses of different constraint methods were both calculated through a three-dimensional coupling thermal-elastic-plastic finite element method and measured by nanoindentation method. The comparison of results indicates that the value of residual stress decreases as the boundary freedom decreases. When the welding specimen is unilaterally restrained, the tensile residual stress appears in the weld fusion line with a peak value of 200 MPa, and the distortion value is 3 mm; when the test piece is applied with full-sided constraints on both sides, the peak value of tensile residual stress appears in the symmetrical

sides of the fusion line with a value of about 100 MPa and the distortion is 1.5mm. The Young's modulus at the elastic phase is 70 GPa and the full elastoplastic material model is sufficient for modelling the material properties of fusion zone in the finite element analysis.

Discontinuous Galerkin method for incompressible two-phase flows

Janick Thomas Gerstenbeger (*Albert-Ludwigs-Universität Freiburg, Germany*) 17:30

Martin Nolte (*Albert-Ludwigs-Universität Freiburg, Germany*)

Samuel Burbulla (*Albert-Ludwigs-Universität Freiburg, Germany, University of Stuttgart, Germany*)

Dietmar Kröner (*Albert-Ludwigs-Universität Freiburg, Germany*)

We consider two-phase fluid flows. The mathematical model is based on the incompressible Navier-Stokes equations with additional jump conditions along the interface, which separates the fluid and vapor phase, and a transport equation for the interface moving with the fluids.

In particular, the interface is tracked by a volume-of-fluid (VOF) method, which keeps the interface sharp and which ensures, that the whole algorithm is mass conservative.

This method is based on a piecewise linear interface reconstruction (PLIC) technique and a 'geometric' flux construction for time evolution.

The incompressible Navier-Stokes equations are discretized in space by a local discontinuous Galerkin (LDG) scheme, where a suitable numerical flux (e.g. local Lax-Friedrichs flux) is used for discretizing the non-linear advection terms.

To sharply separate the fluid and vapor phases special cut-cell quadratures are constructed from the interface reconstructions.

Surface tension is included by integrating the curvature estimates and normals of the interface over the interface reconstructions instead of using a body force formulation like the continuum surface force (CSF).

This surface tension treatment also allows for a simple inclusion of a contact angle boundary condition at the domain bounds.

In this contribution we will present the algorithms and some numerical simulations including some well-known benchmarks and problems with realistic data (water/steam system).

An extension of the presented algorithms to include phase transitions is in works.

Using FEniCS and OpenFOAM for the simulation of conjugate heat transfer in a partitioned fashion

Benjamin Rüth (*Technical University of Munich, Germany*) 17:50

Peter Meisrimel (*Lund University, Sweden*)

Philipp Birken (*Lund University, Sweden*)

Gerasimos Chourdakis (*Technical University of Munich, Germany*)

Benjamin Uekermann (*Technical University of Munich, Germany*)

The simulation of conjugate heat transport (CHT), which is often also referred to as thermal fluid-structure interaction, allows predicting the thermal behavior of solid structures interacting with fluid flow. One example application of high relevance in industry is the simulation of a heat exchanger. Here, the solid acts as a separator of hot and cold fluid and as the transmitter of heat from one to the other. Another example application is the simulation of cooling processes via a cool fluid that streams over a hot machine part.

We choose a partitioned strategy to solve a simple CHT problem, where a hot plate is cooled by a fluid that streams over the hot plate in a channel flow. We use specialized single-physics solvers in the different physical domains: We simulate the heat conduction problem in the solid using

the finite element library FEniCS; the fluid flow and convective heat transport are simulated using OpenFOAM's solver buoyantPimpleFoam for incompressible flow with heat transfer. The coupling library preCICE couples the codes and thus allows the solid and the fluid domain to interact. Adapter codes implement the interfacing between preCICE and the respective solvers. The library preCICE hides the solvers from each other. Thus, the proposed setup is very flexible and single components can be exchanged easily – for example, if a different solver for the solid should be used. FEniCS, OpenFOAM, preCICE and the adapter codes are open-source and freely available.

A Navier-Stokes-Korteweg model for dynamic wetting based on the PeTS equation of state

Felix Diewald (*TU Kaiserslautern, Germany*)

18:10

Michaela Heier (*TU Kaiserslautern, Germany*)

Martin Lautenschläger (*TU Kaiserslautern, Germany*)

Martin Horsch (*TU Kaiserslautern, Germany, Daresbury Laboratory, UK*)

Charlotte Kuhn (*TU Kaiserslautern, Germany*)

Kai Langenbach (*TU Kaiserslautern, Germany*)

Hans Hasse (*TU Kaiserslautern, Germany*)

Ralf Müller (*TU Kaiserslautern, Germany*)

Dynamic wetting of component surfaces can be investigated by finite element phase field simulations.

Often these models use a double-well potential or the van der Waals equation to define the local part of the free energy density at a point of the computational domain. In order to give the present model a stronger physical background the molecular dynamics based perturbed Lennard-Jones truncated and shifted (PeTS) equation of state [1] is used instead. This results in phase field liquid-vapor interfaces that conform to the physical density gradient between the two phases [2]. The model is extended to the dynamic case by a coupling with the compressible Navier-Stokes equations. This coupling requires a tensorial pressure term that complies with the surface tension of the liquid-vapor interface resulting from the PeTS equation of state, comparable to the so-called Korteweg tensor.

A detailed discussion of the model is followed by examples that compare the phase field results to molecular dynamics simulations.

References:

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[2] F. Diewald, M. Heier, M. Horsch, C. Kuhn, K. Langenbach, H. Hasse, R. Müller: Three-dimensional phase field modeling of inhomogeneous gas-liquid systems using the PeTS equation of state, *The Journal of Chemical Physics*, 149(6) (2018) 064701.

S07.03 | Coupled problems

Date: February 20, 2019

08:30-09:30

Room: HS 21

An energetically consistent heat input model for additive manufacturing

Christian Burkhardt (*Friedrich-Alexander-Universität Erlangen-Nürnberg*)

08:30

Dominic Soldner (*Friedrich-Alexander-Universität Erlangen-Nürnberg*)

Paul Steinmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg*)

Julia Mergheim (*Friedrich-Alexander-Universität Erlangen-Nürnberg*)

Additive manufacturing offers the ability to design parts more freely and to realize complex geometries that would not have been manufacturable with conventional processes. In the powder bed-based selective beam melting process parts are built in a layer-by-layer fashion. The building process consists of three repeating process steps, i.e. (i) deposition of a new powder layer, (ii) locally melting areas according to the cross section of the desired part geometry and (iii) lowering of the building platform. For the simulation of the melting process a fine discretization in time and space is usually needed to resolve the energy input adequately and to account for effects like phase-changes. Due to the fact that the cooling process can take time periods between hours and days huge computational costs arise. In the present contribution various numerical models to reduce the computational effort are introduced. Adaptivity in space and time is used to account for the different length and time scales in the process. Furthermore, a temporal integration of the heat input model is used to allow for larger time step sizes. In order to account for possible errors due to the spatial discretization in the heat affected zone, a correction term is introduced, rendering an energetically consistent heat input. Numerical examples show the success of the new numerical strategies.

Simulation of multiphysical coupled Additive Manufacturing processes

Philipp Hartmann (*Leibniz Universität Hannover, Germany*)

08:50

Christian Weißenfels (*Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

In the health care industry a patient specific Additive Manufacturing (AM) of cochlea implants is desirable to improve their functionality. Since a comprehensive understanding of the material behaviour (Room Temperature Vulcanisation medical grade silicon) during the printing process does not exist a simulation driven support of patient specific implant development is necessary. This includes besides the development of a thermochemomechanical coupled large strain curing model the implementation, verification and further development of a suitable meshfree method to accurately predict the extrusion based printing dynamics.

Based on the multiplicative split of the deformation gradient into a mechanical, a chemical and thermal part and an additive split of the free energy into a mechanical and a thermochemical part a large strain curing model is developed. Within this model a process dependent viscoelastic-plastic material behaviour is modelled by a further decomposition of the mechanical deformation gradient.

As a numerical solution scheme a meshfree discretisation of an extended version of the Peridynamics correspondence formulation, allowing the application of the developed material model, is used. Due to the nonlocality of the Peridynamics framework a local-non-local coupling is performed for the resulting thermochemomechanical coupled equations.

In the numerical results the performance capability of the extended correspondence formulation regarding the multiphysical problem is shown. This includes the spreading dynamics and solidification of a curing body under gravitational loading and different temperatures as well as material typical behaviour as shrinkage and the release of exothermic heat.

Finally the applicability of the developed framework for the simulation of an extrusion based AM process is presented.

Influence of electrodeposition parameters on the coating process on open porous media

Christine Grill (*Universität des Saarlandes, Germany*)

09:10

Anne Jung (*Universität des Saarlandes, Germany*)

Stefan Diebels (*Universität des Saarlandes, Germany*)

A growing world population and increasing prosperity cause an increasing demand for energy and raw materials. Raw materials must be used more efficiently to be available for future generations. Application-optimized materials such as cellular media lead to greater sustainability, cost savings and accrued competitive advantages. Foams can be electrochemically coated with a metallic layer to improve the mechanical properties. During the coating process, mass transport limitations lead to an inhomogeneous coating thickness distribution. An inhomogeneous coating thickness distribution also leads to inhomogeneous mechanical properties. The parameters influencing the electrochemical coating process are investigated and the coating process is simulated in this project.

The model describing the electrodeposition process consists of a source term, a sink term, a convection, a diffusion and a migration part, which are linked by the continuity equation. The electrodeposition process influences the coating thickness and the source constant, the velocity, the diffusion constant, the electric field and the sink constant are used as parameters. The influence of the electrodeposition parameters on the coating thickness represent a one side coupling. The influence of the electrodeposition parameters on the coating thickness distribution, is investigated by numerical simulation.

The implementation of the continuity equation is done with C++ by finite differences. The convection part is discretized by a first-order upwind scheme and the diffusion and migration part respectively by a central difference quotient. Source and sink terms are assumed to be linear, therefore the function values at the respective points are used. By investigating the parameters on the electrodeposition process, their influence on the coating homogeneity is studied and homogeneously coated foams with homogeneous material properties can be produced.

S07.04 | Coupled problems

Date: February 20, 2019

08:30-09:30

Room: SR 07

Chemo-mechanical modeling of cathode particles of lithium-ion batteries

Aref Nateghi (*University of Stuttgart, Germany*)

08:30

Marc-André Keip (*University of Stuttgart, Germany*)

Lithium-ion batteries are the most attractive electro-chemical energy storage medium used in portable electronic devices. Recently, they have gained more importance due to their application in hybrid and electric vehicles. In industrial applications of Li-ion batteries, high capacity, long life cycle, safety and low costs of the battery are demanded. The performance of Li-ion batteries might be impaired due to unwanted electro-chemical reactions, leading to capacity loss, self-discharge and thermal runaway. Due to the growing popularity of Li-ion batteries and the complexity of the phenomena involved in their operation, it is important to gain a deeper understanding of the electro-chemo-mechanics of Li-ion batteries.

The intercalation and deintercalation of lithium ions in batteries is a complex interplay of electro-chemical, thermodynamical and mechanical effects. In this work, we discuss a thermodynamically consistent finite strain theory of diffusion of lithium ions in cathode particles. The kinetics of the surface electro-chemical reaction is imposed by the Butler-Volmer equation. The proposed model is numerically implemented using the finite element method and some representative numerical examples are solved.

The interaction of bulk stresses, surface stresses, and diffusion in nanostructured electrodes for lithium-ion batteries

Peter Stein (*Technische Universitaet Darmstadt, Germany*)

08:50

Bai-Xiang Xu (*Technische Universitaet Darmstadt, Germany*)

Nanostructured electrodes have found wide application for lithium-ion batteries. They feature short diffusion paths as well as a large surface area that is accessible to electrochemical reactions. Furthermore, the surface stresses acting on the electrode surface induce a (non-uniform) pressure within the material, providing mechanical stabilization. As a result, nanostructured electrodes exhibit high reversible capacities and stable cycling behavior [1] as well as a higher robustness against mechanical degradation [2]. However, the surface-induced pressure field also affects the electrochemical behavior of the particle, modifying, among other things, surface reaction rates and ionic mobility. In this contribution, we discuss the interaction of surface stresses with the electrochemical behavior of nanostructured electrode particles. We thereby consider ideal analytical shapes, faceted nanoparticles, and regular nanostructures such as inverse opal electrodes. We further demonstrate the impact of surface-stress-induced mechanical fields on defect thermodynamics and kinetics, chemical reactions, and phase transformations.

[1] N. Zhao et al., Pure Appl. Chem. 80:2283-2295, 2008.

[2] C.K. Chan et al., Nat. Nanotechnol. 3:31-35, 2008.

Structural optimization of electrically charged anodes

Stefanie Homberger (*Universität Siegen, Germany*)

09:10

Kerstin Weinberg (*Universität Siegen, Germany*)

Marek Werner (*Universität Siegen, Germany*)

In general, a secondary battery is a multicomponent system composed of anode and cathode material and a separator in between. Within this contribution we will study the anode which is made of graphite or silicon and subjected to a couple of physical effects like thermal expansion, electrical current conductivity, and mechanical deformation. The latest battery developments focus on the design of the anode and try to ensure a safe charging of the electrical device.

However, the design objectives like compliance or conductivity are typically competing against each other. On the one hand, the compliance is adapted as a design objective and is subjected to a minimization condition by applying external mechanical loads. On the other hand, the conductivity is aimed to be maximized. As a consequence there is no global optimum structure. Therefore, univariate optimization of certain objectives is investigated at first. Next, for a bivariate optimization Pareto optimality is used and finite element based numerical simulations are performed. Details of sensitivity analysis, some filtering techniques, and optimality criteria will be presented. The resulting structures will be used for a simulation of the charging process involving multi-field physics.

S07.05 | Coupled problems

Date: February 20, 2019
Room: HS 21

14:00-16:00

Phase-field modeling of electro-mechanically induced fracturing of anisotropic electroceramics

Marc-André Keip (*University of Stuttgart, Germany*)
Ashish Sridhar (*University of Stuttgart, Germany*)

14:00

We discuss the phase-field modeling of fracturing in electroceramics under the action of coupled electro-mechanical loading. Electroceramics are inherently brittle and characterized by pronounced anisotropic properties. In recent years they have proven their increasing utility in a number of industrial applications, most prominently as sensors and actuators. In the present talk, we propose a phase-field approach to modeling crack propagation in electroceramics by means of two different variational formulations acting on different length scales. The first approach considers crack propagation at macroscale at which the electroceramic is characterized by linear piezoelectric behavior. It is based on a three-field problem that couples the mechanical displacement field with the electric potential and the fracture phase field. The second approach considers crack propagation at microlevel at which the electroceramic is characterized by domain patterns. It extends the framework by an additional polarization phase field resulting in a four-field formulation. Both approaches account for anisotropic crack propagation by making use of structural tensors that enter the formulation as additional arguments. The modeling capabilities of the framework are demonstrated by a set of numerical examples in two and three spatial dimensions.

Coupled physics solvers for analysing the magneto-thermal behaviour of a permanent magnet synchronous machines

Abdelhakim Lotfi (*Széchenyi István University Of Applied Sciences, Hungary*)

14:40

Dániel Marcsa (*Széchenyi István University Of Applied Sciences, Hungary*)

Zoltán Horváth (*Széchenyi István University Of Applied Sciences, Hungary*)

Christophe Prudhomme (*Universit de Strasbourg, France*)

Vincent Chabannes (*Universit de Strasbourg, France*)

The main objective of our task is to develop a finite element model to analyse the thermal effects in electric machines during its various operating conditions. The application allows the predictions of simultaneous heat transfer in solid and fluid media with energy exchange between them and to determine the heat removal by natural convection from the machine surface. The permanent magnets and the insulation in the stator windings are sensitive to temperature variations, so a special attention must be paid to this part because the high temperature can affect the durability of the stator winding insulation and the efficiency of the permanent magnets. The prediction of the temperature distribution inside an electric motor is required at the machine design stage in order to control the temperature rise and avoid overheating of the sensitive parts. The accuracy of the thermal model depends on the material properties and the knowledge of losses in electrical machine.

In order to simplify the thermal model, the windings and the stator are treated as homogeneous medium with equivalent thermal parameters and the effective properties to characterize the thermal behaviour are calculated based on the volume-weighted average over all constituents. For heat transfer through the external surface of the machine, natural convection is considered. On the other hand the internal air gap is defined as solid and the effective conductivity to characterize the thermal behaviour of the air gap is calculated from empirical correlations.

This computation is made by coupling transient thermal fields with the developed losses model. The temperature rises with the dissipated electromagnetic losses causing a change in the electromagnetic material properties. The electromagnetic-thermal coupling proposed in this study is a coupling between the transient electromagnetic computation with temperature-dependent material properties, which allows the estimation of the losses distribution of motor, and the 3-D thermal computation, which allows the prediction of the temperature distribution inside an electric motor. The coupling algorithm is based on separately solving of the magnetic field and the heat equations by an individual solution scheme and then exchanging coupling data between the two sub-problems at specific time points.

The 2-D magnetic model is simulated in Maxwell ANSYS software and the thermal model is implemented using the open source Feel++ software. Two examples are presented to assess the accuracy of the developed coupled solvers and the numerical results are compared with the experimental ones, which are obtained from a prototype machine.

Electromechanical coupling in neuron theory

Wolfgang F. Ellermeier (*TU Darmstadt, Germany*)

15:00

The Hodgkin-Huxley or FitzHugh-Nagumo theories of nerve pulse propagation do consider action potential propagation along a nerve fiber by gating action of membrane channels. Recently there has been experimental evidence (T.Heimburg, I.Tasaki) for a thermo-mechanical contribution of the axon membrane's radial, longitudinal and thickness displacements due to phase transition within the membrane material at physiological temperatures, leading to the interpretation of the action potential 'wave of solitonic character'. The coupling remains open to debate and a model for this coupling mechanism is described in the paper.

Coupling nonlinear magneto-thermal problems in frequency domain with the mechanical field

Klaus Roppert (*TU Wien, Austria*)

Florian Toth (*TU Wien, Austria*)

Manfred Kaltenbacher (*TU Wien, Austria*)

15:20

For induction heating processes of thin conducting structures, the frequency of the alternating magnetic field needs to be in the range of 10kHz to 100kHz, depending on the thickness of the

material. Therefore the coupled magnetic-thermal problem shows severe timescale differences between the magnetic and the thermal field, described in [1].

An elegant approach to circumvent this problem is to transform the nonlinear eddy current problem into frequency domain and solve for the steady state solution via a multiharmonic ansatz and harmonic balancing.

We use this method to incorporate the nonlinear magnetization curve into frequency domain and solve the nonlinear eddy current problem for the magnetic vector potential, using edge finite elements. This results in a complex algebraic system, which is solved by a nested iteration strategy, proposed in [2] including an algebraic multigrid preconditioner for edge elements [3].

The thermal problem is considered in its steady state formulation, using a convective diffusive PDE with Joule heating as the right hand side term.

To fully couple the magnetic with the thermal field, the electric conductivity is adapted, according to the temperature distribution of the thermal simulation. After obtaining the temperature distribution, the thermal strain, based on a possibly anisotropic thermal expansion coefficient, can be simulated. The thermal stresses and displacements are investigated, which are crucial for industrial applications, where buckling and plastic deformations must be prevented. The proposed method significantly decreases the computation time, compared to a nonlinear transient analysis, which drastically increases the practical usability.

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Novel mixed finite elements for piezoelectric hysteresis modeling

Martin Meindlhumer (*Johannes Kepler University Linz, Austria*)

15:40

Astrid S. Pechstein (*Johannes Kepler University Linz, Austria*)

Alexander Humer (*Johannes Kepler University Linz, Austria*)

We are concerned with the polarization process in piezoelectric materials. This process is usually described by a set of partial differential equations for the coupled electromechanical problem, e.g., Gauss law of electrostatic and mechanical equilibrium equations. Thermodynamically consistent formulations are based on Gibbs' free energy. Phenomenological models usually comprise of a set of switching and saturation conditions for the onset and saturation of the remanent polarization and strains. The theory of variational inequalities is a powerful mathematical framework to treat certain classes of nonlinear boundary value problems including e.g. hysteretic effects. Well-known examples that can be formulated as variational inequalities are contact problems, plasticity or viscoelasticity. We propose to use variational inequalities to describe electromechanical hysteresis phenomena in piezoelectric materials and present a finite element implementation using phenomenological constitutive models. For this purpose, we use a mixed finite element formulation based on an extension of the TDNNS method for coupled piezoelectric problems. Degrees of freedom for dielectric displacement, electric potential, mechanical stresses and displacements are introduced. For remanent quantities, e.g., the remanent polarization, field variables are added to the set of unknowns. Several examples are presented, such as the (re)poling of piezoelectric material applying an electric field under a certain angle to the polarization and the polarization of a domain with interdigitated electrodes. We compare our results to standard finite element

methods using primal (nodal) degrees of freedom for the electric potential and displacements. For our implementations we use the open source framework Netgen/NGSolve where different element types are provided.

S07.06 | Coupled problems

Date: February 20, 2019

16:30-18:30

Room: HS 21

Phase-field simulations of cracks under dynamic loading

Kerstin Weinberg (*Universität Siegen, Germany*)

16:30

Carola Bilgen (*Universität Siegen, Germany*)

Christian Wieners (*Karlsruher Institut für Technologie, Germany*)

Phase-field fracture simulations have become very popular recently. They are able to address the main challenges in fracture mechanics –the identification of crack initiation and the simulation of the unknown crack paths– in an elegant way.

Our contribution sets the focus on different driving forces for crack growth and on the simulation of waves propagating along the fractured interfaces.

Typically, phase-field methods for brittle fracture employ a variational framework which has been proven to converge to Griffith' classical model. This approach, however, has limits in the pressure dominated regime and therefore we propose ad-hoc driving forces which are motivated physically using general fracture mechanics. Additionally we investigate the effect of the phase-field modeled cracks and interfaces on the propagation of the arising waves. The accuracy and the robustness of the simulation method will be demonstrated with a series of numerical examples.

Modeling of hydraulically induced fractures in elastic-plastic solids

Daniel Kienle (*University of Stuttgart, Germany*)

16:50

Marc-André Keip (*University of Stuttgart, Germany*)

Fracking, i.e. inducing fractures by hydraulic means, is a technique used for extraction of gas and petroleum from rock formations in the subsurface. Thereby a well is stimulated via fractures induced by a pressurized fluid which is injected into the wellbore. This leads to an increased permeability within the deep-rock formations and finally to an increased flow of petroleum and natural gas out of the well. Because of its risks due to environmental issues, such as increased seismic activity or drinking water contamination, this technique is highly controversial in many countries. Numerical simulations can be used to gain a profound understanding of the involved physical processes leading to more precise estimates of associated risks and potentials. Of course, reliable numerical simulations must be based on accurate models and stable algorithms.

Many of the existing models for hydraulically induced fractures are based on the assumption that the solid skeleton undergoes only non-dissipative elastic deformations. However, there is experimental evidence that field measurements (e.g. net-pressure) cannot be described with an elastic material law [1]. Hence we propose a framework that accounts also for dissipative plastic deformations within the solid skeleton. The elastic-plastic material behavior is described by a Drucker-Prager-type plasticity model based on [2] which additionally incorporates isotropic frictional and cohesive material hardening. It is linked to an elastic-plastic failure criterion that drives the fractures. The fractures in turn are modeled by a phase-field approach characterizing a regularization of a crack surface that converges for vanishing length-scale parameter to a sharp crack [3]. Fluid contribution and interaction are incorporated by a Darcy-Biot-type constitutive

formulation [4]. By means of representative numerical examples the model capabilities and performance are demonstrated.

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Hydro-mechanics of fluid-filled fractures - a discussion of numerical coupling schemes

Patrick Schmidt (*University of Stuttgart, Germany*)

17:10

Holger Steeb (*University of Stuttgart, Germany*)

Hydraulic stimulations, i.e. pumping operations are primarily carried out to obtain transient pressure and flux data. Commonly, inverse calculations based on diffusion-based models serve to determine hydraulic properties. Nevertheless, even extended diffusion-based models fail to reproduce hydro-mechanical phenomena which influence the pressure evolution significantly. Immediate non-local volumetric changes due to pressure perturbations act faster than the pressure diffusion within fluid-filled fractures. The difference in time-scale results in inverse water level fluctuations also known as the Noordbergum effect. Besides volumetric phenomena, fracture deformations lead to permeability changes during stimulations and might have a notable impact on the diffusion process. This work uses a non-linear hybrid-dimensional, fully coupled approach designed for fractures with high aspect ratios (length vs. aperture, i.e., $l/\delta > 1000$) to investigate the influence of hydro-mechanical phenomena concerning volumetric and permeability changes. The hybrid-dimensional model is motivated by low Reynold numbers and assumes pressure driven Poiseuille-type flow within fluid-filled fractures that lead to dimension reduction of the fracture domain to a dimension.

A method on aerodynamic load transfer to the flexible car-body of high speed train

Weiyuan Dou (*Beijing Jiaotong University, China*)

17:30

Lele Zhang (*Beijing Jiaotong University, China*)

Facing up to the influence of aerodynamics on a flexible car-body of high speed train (HST) which belongs to a vehicle dynamic system, a method to investigate the elastic vibration of the car-body induced by aero-loads in operating conditions were developed based on a equivalent force system. Simplified aero-loads acting on the car-body were established by using CFD simulations of two trains passing by each other at the same speed of 350 km/h. A reduced degree of freedom model was developed by considering the master nodes in a full-scale model. To carry out the loads on the master nodes of the reduction model, the slave nodes are involved in calculating the equivalent forces (moments) by using a searching strategy of limited neighbor slave nodes. Based on a rigid-flexible coupling model, which includes a flexible car-body, two rigid bogies and suspension systems, simulation was conducted to assess the influence of aerodynamics with considering the track irregularities simultaneously, and its contribution on the elastic vibration

of the flexible car-body was discussed by comparing with a multi-rigid-body model. The results demonstrate the feasibility of the method to introduce the aero-loads to analyze the aerodynamic performance issues of HST with a flexible car-body. This method can benefit from reducing the time consumption in the multi-body dynamic calculation and obtain more information of the elastic vibration of a car-body.

S07.07 | Coupled problems

Date: February 21, 2019

08:30-10:30

Room: HS 21

High-order numerical methods for the thermal activation of SMA fibers

Tobias Gleim (*University of Kassel, Germany*)

08:30

Detlef Kuhl (*University of Kassel, Germany*)

Maximilian Schleiting (*University of Kassel, Germany*)

Alexander Wetzels (*University of Kassel, Germany*)

Bernhard Middendorf (*University of Kassel, Germany*)

An important concept in the improvement and reinforcement of concrete is to adapt its composition for enhanced properties. Ultra-High-Performance-Concrete can be produced with special additives and an improved packaging density. In addition, the strength in the pressure as well as in the tensile region can be brought about by introducing steel fibers. These steel fibers are intended to have certain shapes for improved strength, such as wave shape and or end-hook fibers. The advantage of the mechanical behaviors due to a modified design of the steel fibers is a disadvantage in the production process, since the fresh still liquid concrete can no longer be properly incorporated. Therefore, the idea is to use iron-based shape memory alloys (SMA), because these can be given an advantageous shape, for example straight, during processing and another advantageous shape for the mechanical properties by a change in the final state. SMA's are characterized by the ability to adopt a previously imprinted shape due to thermal activation. This activation temperature would be applied in this case by a thermal aftertreatment, as used for the production of precast concrete products. In addition to experimental investigations, it is crucial to be able to simulate this new generation of concrete with the help of suitable numerical models. In order to be able to correctly predict these highly nonlinear processes during manufacturing as well as in the final stage, high-order methods in space and time are inalienable. The thermal activation in the aftertreatment can be generated either by contact heat over the entire body or by an electromagnetic induction. A simulation of the contact heat can be realized with the aid of the heat conduction equation and a source term at the contact surface. While contact heating results in an overall body heating, an inductive heating process can produce precise heat buildup in the SMA fibers. In order to examine this process, the fully coupled electromagnetic Maxwell equations are combined with the temperature field in a monolithic approach. Both procedures are examined in simulations and evaluated for their advantages and disadvantages with regard to the quality of the final product. The high temperature development leads in the concrete matrix and the SMA fibers to strong temperature-dependent material parameters, which creates a strong nonlinear coupled problem. The main focus of this paper is the development of high-order methods in space and time for the activation of SMA's in a concrete material.

3D virtual elements for finite strain thermo-plasticity

Blaž Hudobivnik (*Gottfried Wilhelm Leibniz Universität Hannover, Germany*)

09:10

Fadi Aldakheel (*Gottfried Wilhelm Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Gottfried Wilhelm Leibniz Universität Hannover, Germany*)

This work outlines an efficient low-order virtual element scheme for the coupled thermo-mechanical response undergoing large deformations. The virtual element method (VEM) has been developed over the last decade and applied to problems in elasticity for small strains and other areas in the linear range. Enlargements of VEM to problems of compressible and incompressible nonlinear elasticity and finite plasticity have been reported in the last years[2,3,4,5]. This work is further extending VEM to problems of finite strain thermo-plasticity [1] and considers details of its numerical implementation using the software tool AceGen [6]. The various formulations presented are based on minimization of energy, with a novel construction of the stabilization energy for the coupled problem. The formulation performance is underlined by means of representative examples. For comparison purposes, results of different finite element discretization schemes (FEM) are also demonstrated.

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Coupled boundary elements and finite elements for applications in thin structures

Michal Pawel Rajski (*RWTH Aachen University, Germany*)

09:30

Maximilian Harmel (*RWTH Aachen University, Germany*)

Roger A. Sauer (*RWTH Aachen University, Germany*)

Finite elements method (FEM) is one of the most popular approaches for solving partial differential equations in computational engineering. It gained that status due to its great flexibility and its broad spectrum of applications. However, to solve 3D problem with FEM the volumetric domain has to be discretized and the numerical integration has to be carried out over the whole domain. This results in sizable systems of linear equations to be solved. On the other hand, boundary element method (BEM) represents the solution of a given partial differential equation as a boundary distribution of its fundamental solution. Therefore, it is only necessary to discretize a given problem only on the boundary, reducing drastically the size of the system of linear equations significantly. In general, each of the methods by itself has its benefits but also limitations, depending on the problems to be solved. Thus, the idea of coupling the BE and the FE method creates a very interesting alternative in a broad spectrum of numerical methods. Multi-physical problems like fluid-structure or electro-elastic interactions can be solved solely on a common curvilinear surface parameterization for boundary element and finite element analysis to admit general surface shapes and deformations. In this work, the BEM formulation for Stokes and Laplace problem is coupled with a nonlinear FE Kirchhoff-Love shell formulation [1] and [2]. Unfortunately, the usage of fundamental solutions in the formulation of the boundary element method causes that the resulting boundary integral equation (BIE) contains singularities in the domain of integration. To address this problem non-singular BIEs are considered [3]. It is shown

that the efficiency of the BEM depends directly on the proper evaluation of the singular integrals. The presented framework is illustrated by numerical examples.

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Lagrangian perspective on multi-scale skeletal muscle models

Steffen Plunder (*TU Kaiserslautern, Germany*)

09:50

Bernd Simeon (*TU Kaiserslautern, Germany*)

In this contribution, we show that the main active contraction stress term in multi-scale skeletal muscle models stems from the coupling of a conservative Lagrangian system with certain constraints. This perspective allows us to view a part of the biological model for skeletal muscles as a Lagrangian system, which implies new numerical objectives and a structure to develop variational integration methods. Muscle cells are composed of parallel filaments, with cross-bridges attached between these filaments. The cross-bridges behave roughly like linear springs and are responsible for the shortening of the muscle cells. Therefore, we model skeletal muscle tissue as a hyperelastic solid, with a collection of linear springs attached at each point of the muscle tissue. The contraction velocity of the linear springs is constrained to be equal to the deformation rate of the muscle tissue in direction of the muscle fibers. With ϕ denoting the deformation field and q the motion of N crossbridges, the Lagrangian of the coupled system takes the form

$$L(\phi, q, \lambda) = L_{elasticity}(\phi) + L_{xb}(q) - \lambda^T g(\phi, q).$$

For N large, it is favorable to describe the crossbridge states by a density ρ_{xb} for the extension of the discrete springs. The second-order equations of motions for q are thus replaced by a first-order transport equation for the density, which might be considered as a master equation of the system. The Lagrange multipliers associated to the constraints are still explicitly given and physically meaningful. This use of densities is advantageous for biological modeling but leads to a mixed system

$$L(\phi = L_{elasticity}(\phi) - W_{active}(\phi, \rho_{xb}), \quad \delta_t \rho_{xb} + v(\phi)\delta_q \rho_{xb} = 0.$$

Such a coupling of a Lagrangian system and a transport equation poses new mathematical and numerical challenges. We discuss appropriate generalizations of variational integrators and present corresponding numerical case studies.

Ingredients for advanced blood damage estimation of medical devices: log-morph with variational multiscales

Lutz Pauli (*RWTH Aachen University, Germany*)

10:10

Stefan Haßler (*RWTH Aachen University, Germany*)

Marek Behr (*RWTH Aachen University, Germany*)

Since several years, our group is developing advanced CFD methods for blood damage estimation of medical devices. Focusing on hemolysis estimation in ventricular assist devices (VADs), which

are small implantable blood pumps for chronically ill heart disease patients, we will present our recent achievements to improve the overall robustness of the simulation workflow.

In our strain-based hemolysis model, the viscoelastic deformation of red blood cells is computed by a morphology tensor. In previous publications (e.g., Refs. [1, 2]), we have already shown that the strain-based model identifies different critical regions in a blood pump if compared to a commonly used stress-based model. Since the morphology tensor computation for state-of-the-art blood pumps remains a very challenging task, we use the matrix logarithm according to Ref. [3] to formulate the so-called log-morph equation. The log-morph equation improves the volume conservation and the overall conditioning of the equation system. Thereby, the new equations allow for larger time step sizes and significantly shorter simulation times in total. For our finite element discretization, we recently derived a residual-based variational multiscale stabilization for the log-morph equation. The multiscale stabilization can improve the solution near no-slip walls, where source terms become dominant.

After introducing the mathematical background, we will discuss the new methods based on simple test cases as well as state-of-the-art VADs. We will also compare our results with experimental data of a benchmark blood pump by the U.S. Food and Drug Administration.

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S07.08 | Coupled problems

Date: February 21, 2019

08:30-10:30

Room: SR 07

Towards multifield discrete element modeling of concrete structures

Christian Flack (*TU Braunschweig, Germany*)

08:30

Dieter Dinkler (*TU Braunschweig, Germany*)

Concrete structures are affected by many external and internal influences during their lifetime. Thus deep knowledge and subsequently mathematical modeling of the different coupled underlying mechanical, physical and chemical processes is extremely important to predict the behavior of materials and structures.

The presented modeling concept is based on discrete element methods and capable of describing processes taking place in the microstructure. The heterogeneous structure of concrete is modeled by a three-dimensional bonded contact model[1], derived from the model of CUNDALL [2] for granular assemblies.

On the meso-scale different phases of concrete have to be taken into account. The aggregates are discretized with rigid spherical particles according to a grading curve. The bond stiffness between the aggregate particles is determined by the cementitious phase. The spring and damper parameters can be adapted to fulfill the global Young's modulus and Poisson's ratio at macro scale. A Voronoi tessellation is applied to create a discrete pore network for transport phenomena. Thermal calculations are performed by a thermal link network connecting the particle centers. The inner structure of concrete is highly dictated by chemical processes during the whole lifetime. The hydration process e.g. is a very complex system of chemical reactions determining strength

and durability at a very early stage. In the present model a process zone is introduced, located between two particles. Within this zone arbitrary chemical reactions can be taken into account. Needed information of concentrations of involved substances are provided by the pore network. Changes in substrates' concentrations lead to variations in the contact stiffnesses due to coupling of processes.

This way a microstructure-related chemo-thermo-mechanical model is developed which may be applied to macro-scale constructions.

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High-performance computational modelling of concrete ageing

Michal Habera (*University of Luxembourg, Luxembourg*)

08:50

Andreas Zilian (*University of Luxembourg, Luxembourg*)

Predictability of the long-term behaviour of concrete construction components is very important for evaluation of structural health and serviceability in the context of continuous system monitoring and life-cycle engineering. The phenomena that must be considered for the mathematical modelling of concrete degradation are complex and lead to coupled multiphysics problems. Such predictive models are challenging not only from the perspective of the involved physico-chemical processes, but also from the computational point of view when robust, reliable and rapid approximate solutions are expected.

In this contribution special attention is given to achieving computational efficiency using a flexible and largely automatised software framework for model discretisation and analysis. The model considered for concrete ageing is based on the microprestress-solidification (MPS) theory of Bazant [1], Kunzel's model for heat and moisture transport [2] and Mazars model for damage [3]. Ageing linear viscoelastic response, which is immanent to MPS theory and concrete creep, leads to ordinary differential equation (ODE) for internal variables solved at every quadrature/nodal point. The accuracy and efficiency of ODE integration schemes and exponential algorithm for internal variables is discussed. For the overall system, Krylov subspace solvers with standard and problem-specific preconditioners are reviewed in terms of convergence properties and condition number. All results are produced within open-source finite element framework FEniCS [4].

The models employed in this study are usually the basis for more involved thermo-hygro-chemo-mechanical (THCM) models with migrating chemical species. It is anticipated, that the presented results can provide helpful indications for the choice of suitable and efficient computational methods for long-term concrete modelling.

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Formulation and calibration of a desorption isotherm for maturing concrete

Peter Gamnitzer (*University of Innsbruck, Austria*)

09:10

Martin Drexel (*University of Innsbruck, Austria*)

Andreas Brugger (*University of Innsbruck, Austria*)

Concrete can be modelled as a porous medium, the pores being filled with moist air and water. In equilibrium, the water content in the pore system is related to the ambient humidity by a constitutive law like relation, the so-called sorption isotherm. The shape of the sorption isotherm depends on the pore size distribution in the porous medium and will therefore change due to hydration. In this contribution, a number of different approaches to model desorption isotherms taking into account changes in the pore structure will be reviewed. These include approaches based on pore space changes caused by hydration and deformation, see [1], [2], for instance. Then, a porosity dependent desorption isotherm for maturing concrete is derived based on an analogy to a deformation based approach [1]. This sorption isotherm is then calibrated using data from quasi-adiabatic calorimetry tests, sorption tests on thin concrete slices, and autogenous shrinkage tests [3]. The determined relation is finally used to simulate early-age drying tests of concrete cylinders. These tests are highly interesting in this context since drying at early age means that states on the sorption isotherm corresponding to high porosity and at the same time low levels of relative humidity are reached, at least close to the drying surface. These states are not accessible during the parameter calibration process, since in the respective tests either the humidity is too high (for the sealed tests) or the porosity is too low (for the sorption tests on the mature slices). However, the drying shrinkage measured on the cylinder is caused by the effective stresses generated right in these locations. Therefore, the results obtained from the drying tests can be seen as an indicator that the assumed sorption isotherm is valid also in these regions.

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Computational modeling of drying shrinkage in early-age concrete

Mehran Ghasabeh (*Middle East Technical University, Turkey*)

09:30

Serdar Göktepe (*Middle East Technical University, Turkey*)

In general, shrinkage is associated with the loss of moisture from concrete in its either fresh or hardened state. At early ages of concrete, when a supply of water is present, continuous hydration process leads to expansion, but when no moisture movement to or from the cement paste is permitted, self-desiccation shrinkage occurs. Beyond this period, isothermal drying of the porous material develops from the variation between the relative humidity of surroundings and the initially uniformly saturated state of the porous medium. The drying phenomenon is a very slow process leading to self-equilibrated stresses and eventually to cracking. Shrinkage-induced cracking can be observed at two scales: at the macroscopic scale where the concrete surface shrinkage is restrained by the concrete core, conversely at the mesoscopic scale, where the cement matrix shrinkage is restrained by the aggregates. Cracking in concrete members accelerate the ingress of water and other detrimental chemical agents, resulting in long-term durability problems such as reinforcement corrosion and sulfate attack.

In the literature, however, there is a limited number of studies on the shrinkage-induced cracking in concrete members where most of the works focus on the experimental study on the relationship between shrinkage and interior humidity of concrete. Most researchers estimate an ordinary shrinkage coefficient, as a linear or hyperbolic function of relative humidity, to associate the shrinkage-induced volumetric strain with the moisture loss by fitting model parameters with experimental results. Therefore, the internal humidity has been traditionally considered as a key field to model shrinkage and shrinkage-induced cracking due to cement hydration and moisture diffusion in concrete while the evolution of volumetric shrinkage strain is determined through empirical expressions.

In this contribution, a hygro-chemo-mechanical modeling of shrinkage in either fresh or hardened concrete is addressed within the framework of poromechanics based on the coupled problem of Darcy-Biot-type fluid transport. In contrast to the previous studies, the so-called water vapor sorption-desorption isotherms are used to relate the mass water content with the relative humidity in calculating the pore pressure as the contribution to the total stress tensor, from which the shrinkage-induced volumetric strain is obtained. The proposed hygro-chemo-mechanical approach is further coupled with a thermodynamically consistent phase field model to predict crack initiation and propagation, induced by shrinkage. Moreover, the consequence of crack growth on diffusivity of hardened concrete is studied to determine the significance of coupling between damage evolution and moisture transport mechanics.

Particle finite element simulation of fresh cement pastes - inspired by additive manufacturing techniques

Janis Reinold (*Ruhr-University Bochum, Germany*)

09:50

Jithender Jaswant Timothy (*Ruhr-University Bochum, Germany*)

Günther Meschke (*Ruhr-University Bochum, Germany*)

The final material properties of concrete structures are dependent on the casting process like filling the formwork or compaction. Hence, to predict the influence of the casting process, it is necessary to understand the flow behaviour of the fresh concrete during casting.

Related issues are faced in techniques, based on additive manufacturing with fresh concrete. In extrusion-based techniques of additive manufacturing with concrete, the mortar or concrete is printed layer-wise to form structural components freely without any use of formwork. Even more than in conventional casting processes, the characteristic properties of concrete components are dependent on the printing process and the time dependent material and flow behaviour.

In this work, a numerical study of additive manufacturing with concrete is performed to analyse the influence of major printing parameters and material properties.

The numerical model is based on the Particle Finite Element Method (PFEM) to simulate the flow of homogenized visco-plastic Bingham-type materials. In PFEM, the governing equations are discretized by means of Finite Elements in an updated Lagrangian framework. Therefore, nodal positions are updated at each time step and a re-meshing is needed to circumvent severe mesh distortions or badly shaped elements.

A velocity-pressure formulation is chosen to solve the balance of momentum and mass. Consequently, for reasons of stability and locking, stable MINI elements with an additional bubble node in the velocity field are used to discretize the system of equations. By static condensation, the bubble degrees of freedom vanish from the system of equations and stabilization matrices naturally appear in the system of equations.

The simplest model to describe the rheological behaviour of fresh concrete is the viscoplastic Bingham model. Due to the non-linearity of the Bingham model, the coupled system of equations must be solved iteratively with a Quasi-Newton method.

In numerical examples of layer-wise printing, the size of yielded regions is assessed and the effects of different printing speeds are analysed. As well, by numerical studies with different

yield stresses and viscosities, thixotropic build-up of concrete at rest is mimicked. Results show that the yield stress is only exceeded in a certain region around the printing nozzle. The size of this region varies with material parameters and printing properties. Hence, shortly after the concrete is being printed, the mechanical behaviour of the material is governed by the regime below the yield stress.

Modeling of active multiphase materials

Malte Sauerwein (*University of Stuttgart, Germany*)

10:10

Holger Steeb (*University of Stuttgart, Germany*)

In this contribution, material modeling and experimental investigations towards a chemically-active multiphase material are presented. The material under consideration consists of a solid skeleton, while the pore space is filled with multiple reactive pore fluids. Here, the pore space is simultaneously filled with a pore liquid and a hydrogel made of a granulate of superabsorbent polymers. The three-phase material is modeled within a continuum mixture theory based on the Hybrid Mixture Theory (HMT). Due to the hydrophilic character, the hydrogel is able to absorb large amounts of the pore liquid and binds it to the polymer structure. As a consequence, the saturation of free liquid in the void space decreases during the absorption, which also affects the permeability with respect to seepage flow. Furthermore, a scenario can be observed experimentally where the hydrogel swells within the pore space to such degree that the fluid flow through the solid matrix comes to a halt. This phenomena is known as gel blocking and used as a self-sealing mechanism for technical applications like self-healing cable sheaths.

Since the absorption dynamics as well as the maximum water capacity of the hydrogel depend highly on external stimuli, e.g. the pore fluid chemistry, temperature, electric and magnetic fields, hydrogels are usually called active or functional materials. The hydrogel material used in this study is sensitive with respect to the ion concentration of the surrounding pore liquid. Experimental investigations have been carried out to capture the swelling behavior of the material for different ion concentrations. The experimental findings are later used to identify model parameters within the continuum-based modeling approach.

The overall idea behind a functional porous material is to control the phase transition within the pore space through external stimuli, namely the transition from free liquid to gel and vice versa. Finally, material parameters like the hydraulic permeability can be controlled indirectly by knowing the constitutive dependence on the gel saturation.

S07.09 | Coupled problems

Date: February 21, 2019

14:00-16:00

Room: HS 21

Modeling the actuation and sensing behavior of an IPMC within the framework of the Theory of Porous Media

Joachim Bluhm (*University of Duisburg-Essen, Germany*)

14:00

Serdar Serdas (*University of Duisburg-Essen, Germany*)

Jörg Schröder (*University of Duisburg-Essen, Germany*)

In the present contribution, a fully coupled electro-chemomechanical model within the Theory of Porous Media (TPM), see Ehlers [1], has been derived in order to describe the material behavior of an ionic polymer-metal composite (IPMC). The considered material consists of fixed anions, attached to the polymer network where both constituents represent the overall solid phase. Additionally, the overall fluid phase is given by an ionic solution (liquid) and the movable cations.

The saturated overall porous medium is assumed to be incompressible. Different motion functions for the solid phase and for each individual constituent of the overall fluid phase are considered. The field equations of the classical thermodynamics in combination with the electrodynamics are discussed, see Markert [2]. Based on the entropy principle, constitutive relations and the corresponding evolution equations have been derived. The established set of the field equations are numerically treated within the framework of the finite element method. In order to represent the main characteristic behaviors of an IPMC, a 1-D numerical example is provided. Therein, the work of Leichsenring et al. [3] is extended by the motion of the liquid phase i.e., the saturation condition is considered. Furthermore, the results of the fully coupled model for the actuation (application of electric potential) and the sensing mechanism (application of displacement) are illustrated by a 2-D problem for a variety of material parameters under a step and a harmonic loading.

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[3] P. Leichsenring, S. Serdas, T. Wallmersperger, J. Bluhm & J. Schroder: Electro-chemical aspects of IPMCs within the framework of the Theory of Porous Media. *Smart. Mater. Struct.*, submitted, 2016.

Interfacial energies depending on curvature: the drastic loss of elastic coupling on small scales and its impact on multiphase mechanics

Patrick Kurzeja (*Institute of Mechanics, TU Dortmund, Germany*)

14:20

The interfacial energy (here: interface energy per unit area) is often assumed to be a constant parameter [2]. Examples include capillarity of water as well as free surfaces of copper nano wires at constant temperatures. The interfacial energy is then typically determined from the energy required to create a planar interface between two bulk phases. Curvature does not enter this notion. It only determines the orientation of the resulting interfacial stresses, for instance, in the famous Young-Laplace equation (capillary pressure = constant interface stress times curvature). This assumption fails, however, when small radii close to the so-called Tolman length [3] are considered. Due to the strong curvature, the plane-interface assumption becomes invalid. Instead, the interfacial energy now significantly depends on the interface's two principle curvatures. The interfacial energy can completely vanish or even change its sign if strongly curved. This is of particular importance for nucleation processes [4]. Even more so, curvature-dependence is a geometrical phenomenon and not limited to specific materials.

The focus of the present investigation lies on the mechanical coupling via curvature-dependent interfacial energies. First, coupling of the curved interface with a bulk sphere and a bulk cylinder is presented to demonstrate its mechanical influence. Namely, mean curvature and Gauss curvature affect different types of mechanical stiffness. Second, a curvature-dependent extension of interface energies up to second order [1,3,4] is introduced to capillary effects around the state of nucleation in continuous and discontinuous mixtures. More specifically, this extension is adapted to wave propagation theory to explore: (i) which length scales are affected by curvature-dependent interfaces and (ii) how can this be detected?

Literature:

[1] W. Helfrich, Elastic Properties of Lipid Bilayers: Theory and Possible Experiments, *Z. Naturforsch.* 28 c, 693-703 (1973)

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Non-locality in multi-scale poroelasticity: phenomena, computational homogenization and numerical model reduction

Ralf Jänicke (*Chalmers University of Technology, Sweden*)

14:40

In heterogeneous porous media, hydro-mechanical coupling between solid matrix and pore fluid under mechanical loading induces fluid pressure gradients and, accordingly, redistribution of fluid in the pore space in terms of a Darcy-type pore pressure diffusion.

In this contribution, we put particular emphasis on the question of non-locality in porous media associated with pore pressure diffusion phenomena. To this end, we interpret the heterogeneous porous rock as a multi-scale material. We coin the name meso-scale for the length scale of heterogeneities (fractures, patchy saturation, ...) which are much larger than the microscopic pores and grains. The hydro-mechanical loading and the overall structural response are assumed to act and to be measured on the macro-scale (separation of scales between micro-, meso- and macro-scale).

In the case of a purely mechanical macroscopic loading, we observe a local redistribution of pore fluid without overall fluid transport. In other words, the diffusion length is, in this case, defined by the typical length of the mesoscopic heterogeneities. Thus, we see that the macroscopic reaction is of viscoelastic nature. If, however, a hydro-mechanical loading is applied on the macro-scale, local fluid redistribution in the pore space is superimposed with a macroscopic fluid transport. This non-local interaction results in an overall poro-viscoelastic material behavior.

In this contribution, we investigate both, the local and the non-local scenario, by computational homogenization. Starting from [1,2] we develop a Numerical Model Reduction (NMR) technique similar to the Nonuniform Transformation Field Analysis (NTFA) to identify the macroscopic (poro-)viscoelastic properties by a set of (“offline“) training computations. This allows us to establish an reduced FE2 scheme to solve macroscopic boundary value problems in a numerically efficient way.

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[2] Jänicke, R., F. Larsson, & K. Runesson [2018]. ‘Identification of viscoelastic properties from numerical model reduction of pressure diffusion in fluid-saturated porous rock with fractures.’ *Comp. Mech.*, DOI 10.1007/s00466-018-1584-7.

A mixed least-squares finite element formulation within the framework of the theory of porous media

Alexander Schwarz (*University Duisburg-Essen, Germany*)

15:00

Solveigh Averweg (*University Duisburg-Essen, Germany*)

Joachim Bluhm (*University Duisburg-Essen, Germany*)

Jörg Schröder (*University Duisburg-Essen, Germany*)

The least-squares finite element method (LSFEM) is an established variational approach in constructing finite element formulations, see e.g. [1]. The method provides some theoretical benefits compared to the well-known (mixed) Galerkin method, since it is not restricted to the LBB-condition. The construction of the finite elements leads to positive definite and symmetric system matrices, also for differential equations with non self-adjoint operators and is applied successfully especially in fluid mechanics, see e.g. [2]. In the present contribution a mixed finite element method based on the Theory of Porous Media (TPM), see e.g. [3, 4, 5], is presented. In

detail we investigate a an incompressible binary model consisting of the phases solid and liquid. The main idea is based on the modelling of saturated porous structures. The resulting finite element is a four field formulation in terms of solid displacements, liquid pressure, mixture stresses and new variable related to the pressure gradient. The conforming discretization of the unknowns in the spaces $H(\text{div})$ and H^1 are realized by vector-valued Raviart-Thomas and standard Lagrange functions. Finally, numerical examples for liquid saturated porous structures considering an incompressible, linear elastic material behavior at small deformations demonstrates the applicability of the LSFEM approach.

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- [2] Z. Cai, B. Lee, and P. Wang. Least-squares methods for incompressible Newtonian fluid flow: Linear stationary problems, SIAM J. Numer. Anal., 42(2):843-859, 2004.
- [3] R.M. Bowen. Incompressible porous media models by use of the theory of mixtures. International Journal of Engineering Sciences 18:1129-1148, 1980.
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The Taylor-least-squares time integrator scheme applied to tracer equations of a sea ice model

Carina Nisters (*Universität Duisburg-Essen, Germany*)

15:20

Jörg Schröder (*Universität Duisburg-Essen, Germany*)

Rainer Niekamp (*Universität Duisburg-Essen, Germany*)

Tim Ricken (*University Stuttgart, Germany*)

The viscous-plastic sea ice model based on [3] describes the motion of sea ice for scales of several thousand kilometers. The numerical model for the simulation of sea ice circulation and evolution over a seasonal cycle includes the consideration of the sea ice thickness and sea ice concentration. The physical behavior of both, thickness and concentration, is described by transient advection equations with the velocity of the sea ice as the coupling field.

Recent research on a finite element implementation of the sea ice model is devoted to formulations based on the (mixed) Galerkin variational approach, compare to [2] and [5] for instance. Here, special treatments are necessary regarding the stabilization of the numerical complex scheme, especially the treatment of the first-order advection equation is crucial in the Galerkin method. It is therefore suggested to utilize the mixed least-squares method, which is well established in the branch of e.g. fluid mechanics, compare to [1] and [4], for instance. A great advantage of the method is its applicability to first-order systems, such that it results in stable and robust formulations also for not self-adjoint operators like for the tracer equations. Moreover, in [6] the authors provide a promising higher-order time integration scheme for transient advection equations denoted as Taylor-least-squares scheme. The presented least-squares finite element formulations are based on the instationary sea ice equations including two tracer equations of transient advection type. The proposed Taylor-least squares scheme is applied to the tracer equations of the sea-ice model and compared to a first-order Crank-Nicolson time integrator scheme for these equations. The different time-integrators are investigated regarding accuracy and stability with a special focus on the treatment of the tracer equations.

- [1] Z. Cai, B. Lee, and P. Wang. Least-squares methods for incompressible Newtonian fluid flow: Linear stationary problems. SIAM Journal of Numerical Analysis, 42(2):843-859, 2004.
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- [3] W.D. Hibler III. A dynamic thermodynamic sea ice model. *Journal of Physical Oceanography*, 9(4):815-846, 1979.
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S07.10 | Coupled problems

Date: February 21, 2019

14:00-16:00

Room: SR 07

FORC measurements - characterisation of interparticle interaction in magnetoactive elastomers (MAE)

Mia Schliephake (*TU Dresden, Germany*)

14:00

Stefan Odenbach (*TU Dresden, Germany*)

Smart hybrid materials offer a number of new applications. By combining the properties of an elastomer matrix system with those of magnetic filler materials new physical properties, like a higher stretch limit of the polymer, are created. The influence of magnetic fillers on a non-magnetic elastomer and the interparticle interaction of magnetic filler components are evaluated by first order reversal curve procedure (FORC) using a vibrating sample magnetometer (VSM). In contrast to major hysteresis loops FORC distributions allow a closer look to the interparticle interaction during the magnetisation process especially when materials show different magnetic characteristics. [1, 2, 3, 4] Additionally the particle movement and reorganisation within the matrix material whilst the sample is exposed to a magnetic field is analysed by 3-dimensional X-ray microcomputed tomography (μ CT). FORC measurements are realised with a Lake Shore VSM on small cylindrical samples with homogeneously distributed particles. Currently the filler components, magnetic hard NdFeB and magnetic soft iron particles, are nestled by a polydimethylsiloxan based polymer matrix. Afterwards the software tool FORCinel generates the mixed second derivative of the magnetisation $M(H_r, H_a)$ with respect to the reversal field H_r and the applied field H_a . Then local magnetisation in every data point is calculated by a second order polynomial fit and in the last step FORCinel plots the FORC distribution after changing coordinates from $M(H_r, H_a)$ to H_c (coercive field) and H_u (interaction field). [1, 2, 3, 4] Furthermore it is important to reduce the data acquisition time by determining the optimal FORC parameters. This is done by modifying field increments, averaging time, time constants and maximum applied field strength. Summarising the results an optimal magnetisation curve is given at small field increments in combination with at least 2s averaging time. Additionally first interesting results were found at an applied field strength of approx. 1600kA/m. A close observation of the magnetisation curves reveals unexpected deviations from the typical hysteresis loop in form of curve crossings and divergences in the forward and backward sweep. In the following, it is of great interest whether this behaviour is due to a previously unprecedented magnetisation effect of the of the magnetoactive elastomer.

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Viscosity increase caused by anchoring of functionalized magnetic nanoparticles in nematic liquid crystals

Josefine Jahn (*Technische Universität Dresden, Germany*)

14:20

Stefan Odenbach (*Technische Universität Dresden, Germany*)

The molecules of thermotropic nematic liquid crystals (LC) are orientated parallel and build a ordering caused by the dipole moments of the molecules. Thus, they are self-organized materials which combine fluid-like behaviour and anisotropic physical properties depending of the temperature [1,2]. Exceeding the phase transition temperature, the thermal motion of the molecules causes a sudden decrease of the ordering and induces an isotropic state. The doping of LCs with functionalized magnetic nanoparticles leads to an interaction between these particles and the LC [3]. This modifies the mechanical flow characteristics and rheological investigations of a doped nematic phase show a viscosity increase, which is significant higher than the theoretical expected one.

Investigated were the pure nematic LC 4-Cyano-4'-pentylbiphenyl (5CB) and 5CB doped with 0.019 vol% $CoFe_2O_4$ -particles (core diameter 2.5 ± 0.6 nm). These particles were functionalized with (pro)-mesogenic ligands of 16-((40-Cyano-[1,10-biphenyl]-4-yl)oxy)hexadecanoic acid. Pretests have shown a phase transition at 307.5 K. The viscosity was measured in a rotational rheometer with a cone-plate geometry (diameter 25 mm). The shear rate was varied from 1/s to 100/s and the isotropic state was measured at 293 K, the nematic state at 313 K.

Isotropic 5CB has a Newtonian behaviour [4,5] and the viscosity is independent of the shear rate, however nematic 5CB has shown a shear thinning behaviour which follows a power law approach. The following viscosity increases were measured: $\Delta\eta/\eta$ (isotropic) = 4.59 p, 0.91 % and $\Delta\eta/\eta$ (nematic) = 6.32 % (R^2 of regression curves > 81 %), respectively calculated according to the Einstein equations [6]: $\Delta\eta/\eta = 0.0475$ %.

In the isotropic and nematic state of 5CB the Einstein equations does not apply because the cyanobiphenyl entities of the ligands interact with the LC-molecules which leads to an anchoring of the particles in the LC-host. Thus, the fluid can no longer be considered as a continuum respectively to the particles. Since the interaction mechanisms between the dipolar LC-molecules among each other and between the LC-Molecules and the magnetic particles are still poorly understood [3], simulations, where the particles and the LC-host interact via a generalized Gay-Berne potential [7-9] can help understanding these mechanisms.

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Coupling and computation of electromagnetism and mechanics

Bilen Emek Abali (*Technische Universitaet Berlin, Germany*)

14:40

Electromagnetic fields apply a (ponderomotive) force on the structure such that the underlying body deforms. Simultaneously, a deformation causes moving electric charges inducing electromagnetic fields. An accurate coupling of electromagnetism and mechanics is very challenging because of two distinct reasons. First, from a theoretical point of view, there is a mismatch in classical theories between the transformation properties of governing equations, namely Maxwell equations for electromagnetic fields and balance equations for mechanics. Second, by means of modeling polarized materials, we simply fail to know the correct formulation of this ponderomotive force. This lack of definition is often called the Abraham–Minkowski controversy. We need an accurate computation of displacement and electromagnetic fields in order to be able to perform simulations and inspect different suggestions for modeling the ponderomotive force. Hence, in this talk, we follow the framework presented in [1] and present the computation of electromagnetic fields and deformation by means of the finite element method in a way that the coupling is being captured accurately.

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Development of a macro-model for magnetorheological elastomers based on microscopic simulations

Karl A. Kalina (*TU Dresden, Germany*)

15:00

Philipp Metsch (*TU Dresden, Germany*)

Jörg Brummund (*TU Dresden, Germany*)

Markus Kästner (*TU Dresden, Germany*)

Magnetorheological elastomers (MREs) are a class of active composites which consist of a soft polymer matrix with embedded micron-sized magnetizable particles. Due to strong magnetic interactions of the embedded particles and the resulting deformation of the matrix, MREs are able to alter their effective mechanical properties if an external magnetic field is applied.

In this contribution, we present a microscopic modeling approach [1,2,3,4]. Starting from the properties of the magnetizable particles and the elastomer matrix, a magneto-mechanical continuum formulation is applied. The governing equations of this strongly coupled field problem are solved by a nonlinear finite element formulation. By performing computational homogenizations [1,3,4] for different random microstructures, the microscopic model is used to predict the macroscopic behavior for different effective load states of the considered MREs numerically.

With the aid of the generated simulation data, a thermodynamically consistent macro-model for isotropic MREs is developed in a systematic way. Finally, the unknown parameters of the nonlinear model are identified incrementally by applying several least square fits based on these data. The developed model is used to simulate macroscopic MRE samples and structures.

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Coupling of a peridynamic continuum with an analytical solution

Moritz Becker (*Technische Universität München, Germany*)

15:20

Peridynamics is a nonlocal formulation of continuum mechanics which uses integral equations for the balance of momentum and an internal length scale called the peridynamic horizon. Therefore, the theory is able to deal with discontinuous displacement fields and shows dispersive behavior. The peridynamic equation of motion can be solved by a finite element approach also. Investigated is a 1-D elastic bar split in two regions. One region is discretized with peridynamic finite elements. Coupled to this region is a 1-D classical continuum, for which an analytical solutions can be derived. In the scope of this talk, the coupling of both regions is presented. Subsequently investigated is the influence of the length of the peridynamic horizon in the coupling region and the dispersive effect of the peridynamic waves on the solution. The results are compared to a Finite Element analysis.

S07.11 | Coupled problems

Date: February 21, 2019

17:40-18:40

Room: HS 21

Determination of material parameters for a multiphasic modeling of hydrogels

Beatrice Mau (*Technische Universität Dresden, Germany*)

17:40

Jan Erfkamp (*Technische Universität Dresden, Germany*)

Margarita Günther (*Technische Universität Dresden, Germany*)

Thomas Wallmersperger (*Technische Universität Dresden, Germany*)

Stimuli-responsive hydrogels are electroactive polymers classified as smart materials, consisting of a solid, fluid and ionic phase. As a result of external stimuli, for example through a variation of the chemical conditions in the surrounding solvent, the hydrogels undergo a reversible volume transformation caused by the absorption or the release of solvent. By using a multiphasic model based on the Theory of Porous Media the chemo-electro-mechanical interaction of the different phases can be described. Therefore this model requires a large amount of material parameters, whose determination poses a challenge. To determine the parameters for the mechanical behavior it should be ensured that an interaction of the different phases (solid and fluid) and the surrounding solution bath is realized in order to investigate the viscoelastic behavior of the hydrogel. In the present research, a tensile test is performed to identify the mechanical properties of such stimuli-responsive hydrogels. Therefore, a specific focus is placed on the dependence of these properties on the solid-fluid ratio due to the multiphasic composition of this material. The aim of this research is to ameliorate the material equations of the modeling and consequently enhance a prediction of the mechanical behavior.

A finite element analysis of a coupled diffusion-deformation theory for elastomeric hydrogels

Aidin Hajikhani (*Leibniz University of Hannover, Germany*)

18:00

Michele Marino (*Leibniz University of Hannover, Germany*)

Peter Wriggers (*Leibniz University of Hannover, Germany*)

Hydrogels are attracting enormous attention in nanotechnology because of their perceived intelligent behaviour. They can be utilized as scaffolds, or nanoparticles in various biomedical and

biological applications such as bioprinters, and drug delivery. Recent 3D bioprinting technology allows us to print three-dimensional scaffolds where living cells are embedded in biocompatible materials. Due to its biocompatibility and relatively low cost, alginate hydrogel is a natural polymer which has been extensively used as bio-ink for the production of scaffolds for cell growth, division, and reproduction. Alginate hydrogel undergoes mild gelation by adding an ionic stimulus (cross-linker) such as Calcium ions which stabilizes the polymer network via cross-linking [1]. In bioprinting applications, the solvent is combined with the aqueous alginate solution. This work addresses the secondary cross-linking where the solvent is poured on the printed specimen. The diffusion of the solvent in the hydrogel during the gelation process stabilizes the polymeric network. This process will produce inelastic deformation, in turn, responsible for residual stresses and will affect the final scaffold geometry and the cell behaviour inside the biomaterial. Consequently, the structural resolution, shape fidelity and cell survival depend on properties and characteristics of the bio-ink during the gelation process. This work aims to develop a computational model of the gelation mechanism in alginate hydrogels. The chemo-mechanical system consists of elastic, shrinking and swelling mechanical deformations promoted by the chemical potentials of the cross-linker and the fluid content. Hence, the chemical potential of the cross-linker and the fluid content govern the shrinkage and swelling inelastic strains, respectively, on the hydrogel. Thereafter, a constitutive model is developed, considering the influence of the cross-linker and the fluid contents on the deformation gradient of the shrinking and swelling phenomenon. Consequently, the developed computational framework allows to quantitatively predict stress distribution inside the hydrogel as a function of internal chemical reaction[2]. Numerical approaches for multiphysics mechanisms have been developed and implemented in a finite element framework, considering the monolithic coupling of chemical transport and mechanics [3]. The benchmark test validates the computational framework which is calibrated towards the experimental data. The importance of accounting the coupling effect between the shrinking and the swelling phenomenon is highlighted, showing the effectiveness of the proposed model.

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An overview of simulated hydrogel behaviour under various kinds of stimulation

Karsten Keller (*Universität Stuttgart, Germany*)

18:20

Thomas Wallmersperger (*Technische Universität Dresden, Germany*)

Tim Ricken (*Universität Stuttgart, Germany*)

The auto-responsive behaviour of hydrogels, crosslinked polyelectrolytic polymers embedded in aqueous solution, show effects under various kinds of stimulation. These changes of the environmental conditions could be e.g. of chemical, electrical, mechanical and thermal nature. These hydrogels react via uptake or delivery of mobile ions and solvent, and they show enormous swelling capabilities. This multifunctional behaviour is potentially attractive for chemo-electro-mechanical energy converters or for the use as actuators or sensors. In the present research anionic and cationic hydrogels are investigated, which means the polymer network includes anionic or respectively cationic bound charged groups. The investigated stimuli are chemical, electrical, mechanical, and thermal. The chemical stimulation is applied by the change of boundary conditions e.g. of the constituents themselves (Na^+ and Cl^-) or for the pH-stimulus by investigating further species ($\text{H}^+/\text{H}_3\text{O}^+$ and OH^-) plus dissociation reactions. To model the electrical stimulus we incorporate electrodes on which a transient electric potential is applied. The mechanical stimulus is defined by prescribed displacements at a boundary of the hydrogel itself. The thermal stimulus is applied as transient temperature change over the whole domain incorporating temper-

ature dependent material parameters. The hydrogel mechanical/ non-mechanical answer differs depending on the stronger or weaker sensitivity to the applied stimulus. The fully coupled three field description of the chemo-electro-mechanical model enhanced with thermal dependencies is capable of giving local concentrations, electric potential and displacements. All four types of stimulation are applied independently and the results are demonstrated for different configurations. Acknowledgements: This research has been financially supported by the Deutsche Forschungsgemeinschaft (DFG) in the framework of the Priority Programme 1259 (SPP) Intelligente Hydrogele under the grant number Wa 2323/2.

S07.12 | Coupled problems

Date: February 21, 2019

17:40-18:40

Room: SR 07

Multiphysics modeling and simulation of fluid-saturated porous ferrogels at finite strains

Philipp Gebhart (*TU Dresden, Germany*)

17:40

Thomas Wallmersperger (*TU Dresden, Germany*)

Over the last years there has been a growing interest in the study of the behavior of field-responsive or so called smart materials. Porous ferrogels are a special class of these materials consisting of a porous polymeric matrix with dispersed micro- or nano-sized ferromagnetic particles [1, 2]. Due to their ability to exhibit large deformations and alter their effective material characteristics upon external magnetic stimulation, these materials are interesting for a wide range of applications in biomedical engineering, microfluidics and other innovative fields of research.

The magneto-poro-mechanical response of porous ferrogels is a complex phenomenon that spans over multiple length-scales and essentially depends on (i) the constitutive behavior of the individual components, (ii) their microstructural arrangement and (iii) the macroscopic shape of the specimen. In this contribution a theoretical and computational framework for the modeling of isotropic porous ferrogels at the macroscale is presented. Within our modeling approach the porous ferrogel is treated as a homogeneous continuum, whereat its complex microstructure is not resolved explicitly. A prototypical constitutive model is formulated in a conventional enthalpy-based setting according to [3]. In order to preserve an adequate mesh quality in the free space surrounding the ferrogel a mesh-morphing algorithm is employed, which is sufficiently robust for finite deformations.

Numerical examples demonstrate the capabilities of the framework and show the crucial impact of the macroscopic specimen shape on the homogeneity of the magnetic and mechanical fields in an uniform external magnetic field.

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A coupled thermo-hydro-mechanical model with double porosity for plant tissues

Lukas Eurich (*University of Stuttgart, Germany*)

18:00

Shahla Shahmoradi (*University of Stuttgart, Germany*)

Arndt Wagner (*University of Stuttgart, Germany*)

Ronaldo Borja (*Stanford University, USA*)

Wolfgang Ehlers (*University of Stuttgart, Germany*)

Many plants have developed fascinating strategies to cope with multiple cycles of freezing and thawing events without being damaged. Understanding the involved strategies and mechanisms of plants exposed to subfreezing temperatures is of high interest, as they could potentially be used for the development of bio-inspired construction materials with optimised properties in terms of frost resistance, thermal isolation and guided water or moisture transport.

With regard to frost resistance of plants, the dehydration of their tissue cells is a key factor, as a lower water content within the cells leads to a lower freezing point of the intracellular water. Thereby, intracellular ice formation can be avoided, which is crucial for the survivability of the plant. Since the cell dehydration is a consequence of coupled thermo-hydro-mechanical processes, a modelling approach based on the Theory of Porous Media (TPM) is applied, describing the multiphasic aggregate on the macroscale. In particular, the porous plant tissue is modelled by a ternary model consisting of the tissue cells, which are themselves a porous material composed by solid tissue material and (initially) trapped water. Therefore, the dehydration of the cells is governed by the micro-porosity of the cell membrane. The intercellular space is filled with two pore fluids, namely air and water. This allows for a thermodynamically consistent description of the cell dehydration, which is as mass production term in the respective balance equations included.

Within the scope of this contribution, the effect of ice formation at the exterior surfaces is considered. It has been reported for the *Equisetum hyemale*, the plant under current investigation, that ice formation occurs in the pith cavity and even more pronounced in the so-called vallicular canals, which are large gas-filled compartments. This is taken into account by imposing appropriate boundary conditions at these surfaces, which leads to a pore-water flux towards these surfaces and a dehydration of the tissue cells due to a change of the chemical potential of the pore water. Numerical results show qualitatively the experimentally observed behaviour, i.e. the mass interaction of water and its efflux from the porous tissue material into the gas-filled compartments, which eventually may freeze.

Modelling of ice formation and brine flow in Antarctic sea ice in the framework of the extended Theory of Porous Media (eTPM)

Andrea Thom (*University of Stuttgart, Germany*)

18:20

Tim Ricken (*University of Stuttgart, Germany*)

According to NASA (National Aeronautics and Space Administration), Antarctic sea ice has reached its lowest extent ever recorded by satellites at the end of summer 2017 in the southern hemisphere after decades of moderate sea ice expansion. Besides a strong influence on the global climate linking the exchange of energy and gases between the atmosphere and the ocean, changes in sea ice have also a biological response concerning the ecosystem structure and function. These responses are strongly related to the physical and mechanical properties of the sea ice structure. Seawater is trapped in so-called brine pockets during the growth of sea ice, providing a natural habitat for sea ice microorganisms. The microorganisms are supplied with nutrients from the seawater they need for primary production. A small-scale modelling of the porosity of the sea ice

and its inclusions and the solid/brine multiphase microstructure, respectively, thermodynamics of air-sea interactions as well as sea ice-biological linkages is a necessary tool to understand the heterogeneous sea ice nature better.

Based on the extended Theory of Porous Media (eTPM) [1, 2], the development of a multi-phase, multi-component model which enables the continuum mechanical description of transport and phase transition phenomena in sea ice at a homogenized pore scale is presented. The model consists of a solid (ice) and liquid (brine) phase including dissolved nutrients in brine. Within this framework, thermodynamical consistent model formulations for the natural convection of the saline brine and its impact on the nutrient supply and primary production by ice algae are developed.

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S07.13 | Coupled problems

Date: February 22, 2019

08:30-10:30

Room: HS 21

Simulation of thermoelastic problems with the finite element method

Fabian Matter (*Universität Stuttgart, Germany*)

08:30

Pascal Ziegler (*Universität Stuttgart, Germany*)

Peter Eberhard (*Universität Stuttgart, Germany*)

Disc brakes have the task to convert kinetic energy into thermal energy and so to slow down a vehicle. During the braking process enormous heat flows and temperature gradients can occur in the system. Because heating leads to a change in shape for most materials, it is important to take the temperature and its influence into account in the design process. The interaction between the structure and the heat in disc brakes can be described with methods from thermoelasticity. To simulate thermoelastic behaviour the Finite Element Method is commonly used. The thermal and the mechanical domain are taken into account by coupling the equation of motion and the heat equation. However, in transient analysis occurs the problem of different time scales of the structural and thermal dynamics for many technically relevant materials, like steel. For metallic materials the time constant of structural dynamics is much smaller than those of thermal dynamics. This complicates an efficient transient simulation.

In the present work the implementation of a Finite Element Method in thermoelasticity and associated investigations are shown. The method is applied on various parts and load cases. Also different approaches to deal with the different time scales will be shown. Physical methods like mass-scaling as well as more mathematically oriented approaches like model order reduction will be presented.

Finite-strain thermo-viscoplasticity for case-hardening steels over a wide temperature range

Philip Oppermann (*Lund University, Sweden*)

08:50

Ralf Denzer (*Lund University, Sweden*)

Andreas Menzel (*Lund University, Sweden, TU Dortmund, Germany*)

The aim of this work is the development of a thermodynamically consistent fully coupled thermo-viscoplastic material model for metals undergoing finite deformations.

A multiplicative split of the deformation gradient into a thermal, an elastic and a plastic part is introduced, where isotropic thermal expansion and isochoric plastic deformation are assumed. The model is based on a decomposition of the free energy into a thermo-elastic and a plastic part and covers non-linear cold-work hardening and thermal softening. The model incorporates non-linear temperature dependent effects for the elastic moduli, thermal expansion, heat capacity, and heat conductivity. Furthermore, the temperature and strain-rate dependency of the yield stress is realised using a Perzyna-type viscoplastic model incorporating a von Mises yield function, both enhanced by thermal softening. Special care has been taken for the time integration of the plastic deformation gradient to comply with the incompressibility constraint. The model and its parameters have been fitted against experimental data for case hardening steel 16MnCr5 (1.7131). We discuss the consistent linearisation of the proposed model and its implementation in a monolithic fully coupled finite element framework. Finally, we present results for selected boundary value problems. They show the localisation and regularization behaviour of the proposed model.

A diffuse-interface model for two-phase flow with thermocapillary effects and phase transitions

Ivan Yashchuk (*VTT Technical Research Centre, Finland*)

09:10

Selective Laser Melting (SLM) is an Additive Manufacturing (AM) process. During SLM process a laser is used to melt metal powder particles and build parts layer-by-layer.

In this contribution, we present a phase field model for powder scale melting and solidification of metal including dynamics of liquid-gas interface and associated (thermo-)capillary effects. The governing PDE system consists of the Navier-Stokes equations coupled with convective phase-field and energy transport equations, in which the material parameters are allowed to be temperature and phase dependent functions. The proposed model is implemented using FEniCS and the resulting nonlinear system is solved monolithically. Appropriate numerical examples that showcase the capability of the proposed model to capture different phenomena of the AM process are presented.

Hygro-micromechanical analysis of the interfiber bonding in a fiber-network

Binbin Lin (*TU Darmstadt, Germany*)

09:30

Functional paper materials have attracted research attention for sensor applications, and chemical and consequently mechanical modifications of fiber-fiber bonds are introduced. For the processibility and serviceability, the mechanical property and durability of papers are vital, both of which strongly depends on the properties of the constituent fibers, fiber-fiber bonds and fiber network with microscopic details. A model allowing direct access to these microscopic aspects is indispensable.

Paper is, essentially, a network of cross-linked cellulose fibers. Besides the individual fibers' mechanical properties, the interfiber bonding at the microscopic level plays an essential role for the extensibility and strength of the considered paper material. Local stiffness reduction/change in the fiber-interface due to moisture uptake and hygro-expansion leads to inhomogeneous stress distribution and lowers the strength of paper. This contributes to fatigue of the material or even to fracture initiation.

This study is concerned with a hygro-micromechanical analysis of the interfiber bonding of two fibers when they are torn apart. The fiber geometry and interface contact area are thereby obtained from image data. We employ a cohesive zone model for the inter-fiber interface and

analyze the mechanical behavior with respect to different relative humidity. Mechanosorption, describing the response of fiber-interface due to the interaction of moisture change and mechanical tension will be studied. The moisture transport from the environment will be analyzed using a transport equation coupled to the mechanical analysis. The results will be used to predict the long-term mechanical behaviors of used paper-structure.

Polymorphic uncertainty quantification of computational soil and earth structure simulations via the variational sensitivity analysis

Carla Henning (*University of Stuttgart, Germany*)

09:50

Tim Ricken (*University of Stuttgart, Germany*)

The design security concept of earth structures requires very high safety factors in contrast to industrially manufactured materials like steel or concrete. This is caused by natural scattering of material properties, the very high complexity of the soil structure on different length scales and the load bearing mechanism as well as the residual stress state due to individual load histories. Reliability assessment of soil structures and suitable numerical methods for computational simulations still poses considerable challenges for industry and science. By means of increasing computing power and enhanced mathematical models, a better understanding of the nature and influence of the uncertainties and errors could help to develop a more reliable risk assessment and to reduce inefficient safety factors.

For this aim, we perform a research project within the priority program SPP 1886, installed by the DFG and focused on polymorphic uncertainty quantification. In the present subproject (SP 12), the focus is driven on quantification and assessment of polymorphic uncertainties in computational simulations of earth structures, especially for fluid-saturated soils.

To describe the strongly coupled and transient solid-fluid response behavior, the theory of porous media (TPM) is used and solved via finite element method (FEM) [1, 2]. Motivated by structural optimization research, the variational sensitivity analysis (VSA) provides detailed information about the current equilibrium state not only with respect to the unknown variables but also to variations in material parameters or boundary conditions. In this work the methodology is transferred to quantify uncertainties, see Henning and Ricken [3]. The method enables an immediate decision support, e.g. for site investigators. Not only the computational effort but also the applicability to any arbitrary FE-Model are great advantages of this approach. It provides a lot of additional information for end-users as well as researchers.

After discussing the basic framework, governing equations and algorithmic implementation of the proposed model, the applicability will be demonstrated by simple boundary value problems.

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Optimization of diffusion driven degradation processes

Navina Waschinsky (*TU Dortmund, Germany*)

10:10

Franz-Joseph Barthold (*TU Dortmund, Germany*)

Andreas Menzel (*TU Dortmund, Germany*)

It is known that the nature always aims for optimal processes, for example bones which regulate the tissue in areas of high stresses or the optimal shape of trees which prevent early failure. Due to the permanent competition in nature, it has developed intelligent optimization algorithms

which regulate underlying decay processes. We are taking nature itself as a role model in order to think of optimization processes in civil engineering for structures which suffer from destructive influences for example chemical attacks.

We will focus on biologically-inspired degradation processes which are often accompanied by nutrients interactions. Thereby tissue elements continuously receive additional mass or release mass due to diffusion phenomena. The continuum mechanical theory is used to describe the coupled aspects between mechanics, diffusion and mass creation/resorption. With a thermodynamically consistent formulation of a single-phase open system we will evaluate the constitutive equations for the stresses, mass source and the evolution of growth. The diffusion is a gradient-based formulation of nutrient motion in analogy to Fick's law. Thus, chemical reactions of specific nutrients trigger degradation and growth processes leading to large deformation. A multiplicative decomposition of the deformation gradient in an elastic and growth part will be used as the kinematic approach for volumetric growth. For simplicity we will focus on isotropic growth. The outlined continuum mechanical theory will be embedded in an optimization algorithm thereby the destructive process of mass degradation can be minimized.

As a representative example for the application of the theory we will discuss calcium leaching in concrete. Calcium leaching is a material deterioration which often appears in concrete due to elusion of calcium when long-term contact with water is given. However, a civil structure consisting of concrete is designed to have a long lifetime. With an optimization algorithm of the degradation process we can evaluate the optimal geometry of a structural component which ensures stability despite destructive influences of degradation of mass.

S07.14 | Coupled problems

Date: February 22, 2019

08:30-10:30

Room: SR 07

A finite-element framework for the modelling and simulation of phase transforming magnetic solids using energy relaxation concepts

Thorsten Bartel (*TU Dortmund, Germany*)

08:30

Björn Kiefer (*TU Bergakademie Freiberg, Germany*)

Andreas Menzel (*TU Dortmund, Germany, Lund University, Sweden*)

The macroscopic behaviour of ferroic functional materials such as magnetic shape memory alloys (MSMA) is highly affected by microscopic mechanisms such as the formation and further evolution of microstructures. Thus, the modelling of these effects is important for establishing micromechanically well-motivated constitutive frameworks with high physical plausibility. In this contribution, a general and comprehensive Finite-Element-based modelling framework is presented where the switching between different crystallographic variants of martensite as well as the propagation of magnetic domains is treated by the evolution of phase volume fractions on the basis of energy relaxation methods. In addition to these mechanisms, possible deviations of the local magnetisation vectors with respect to the easy axes also need to be taken into account in order to simulate the material behaviour accurately. For homogeneous problems (e.g. elliptic bodies), the influence of the demagnetisation field can be captured by demagnetisation tensors and the effective quantities such as stresses and the magnetic induction can be calculated in a post-processing step. For inhomogeneous problems, however, the demagnetisation field has to be treated as an independent field variable. In this context it can be stated that conventional Finite-Element-based implementations, where internal state variables are locally determined at the integration points in a condensed manner, are hardly, if at all, realisable. Thus, the variables describing the microstructure are also treated as global field variables and the related Biot-type evolution equations are solved at the macroscopic level. In this contribution, the theoretical

approach as well as the Finite Element implementation will be elaborated, the latter being supported by illustrative examples of the fully magnetomechanically coupled behaviour of materials, such as MSMA response.

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Modeling and simulation of magneto-elastic coupling using FFT-based homogenization methods

Felix Dietrich (*Technische Universität Kaiserslautern, Germany*)

08:50

Mané Harutyunyan (*Technische Universität Kaiserslautern, Germany*)

Magneto-elastic coupling describes the mutual dependence of elastic and electromagnetic fields and can be observed in certain types of materials, among which are the *magnetostrictive materials*.

On the one hand, these materials experience a strain or deformation when an external magnetic field is applied (*magnetostriction*). On the other hand, their magnetization is changed when they are subjected to mechanical stress (*inverse magnetostriction*). Due to their remarkable properties, magnetostrictive materials have wide application areas: They are used as variable-stiffness devices, as sensors and actuators in mechanical systems or as artificial muscles in robotics.

The aim of our work is the mathematical modeling and numerical simulation of the magneto-elastic coupling in magnetostrictive materials on a microscopic level using spectral solution methods. These have gained the attention of many researchers over the past years with one of the pioneering and most cited works being the *Basic Scheme* developed by Moulinec and Suquet. Its advantages consist of being directly applicable to given image data without an additional meshing step, as well as a matrix-free and straight forward implementation. To this end, a homogenization assumption is made, allowing for the *Fast Fourier Transform* to be used on a local scale to solve for effective material properties. Since its introduction, the algorithm has seen numerous variations and has been extended to multiple problems and material classes.

Our work focuses on two main aspects: First, we derive and analyse a coupled magneto-elastic model for magnetostrictive materials under the assumption of a linear and reversible material behavior. Second, we aim at the application of spectral methods to the obtained coupled system of partial differential equations using the Basic Scheme of Moulinec and Suquet.

The interplay of particle structure and mechanical properties in NdFeB-loaded magnetorheological elastomers

Malte Schümann (*Technische Universität Dresden, Germany*)

09:10

Julian Morich (*Technische Universität Dresden, Germany*)

Stefan Odenbach (*Technische Universität Dresden, Germany*)

Magnetorheological elastomers are a class of smart materials. Here, the embedment of magnetic microparticles in an elastomeric matrix leads to the ability to control the mechanical behavior of those materials by the application of external magnetic fields. A key to gain a deeper understanding of magnetorheological elastomers is the analysis of the internal particle structure which determines the macroscopic material behavior to a great extent.

For this study a magnetorheological elastomer with 40 wt% of highly anisotropically shaped NdFeB particles was synthesized. The particle structure and the magnetically induced motion of the particles was evaluated by means of X-ray microtomography. The sample was gradually magnetized up to an external field of 2 T. At each point of magnetization a 250 mT field was applied during tomography and mechanical testing.

The successive magnetization up to 2 T leads to a transition from the initial isotropic particle distribution to particle chains. The application of the 250 mT field results in a distinct rotation of the single particles. A mostly reversible alteration of the particle structure was observed at low magnetizations. Higher magnetizations lead to a non-reversible chain formation of the particles. The pair correlation function offers a convenient method to analyze the arrangement of particles based on their positions [1]. For this work, a direction dependent implementation of the pair correlation function was applied to evaluate the anisotropy of the particle structure. This method enables to determine the point of commencing chain formation. At a certain external magnetization the formation of an anisotropic particle structure begins. At this stage a significant change in mechanical properties was observed as well. Accompanying mechanical characterizations show a significant magnetorheological effect, an increase of the Young's modulus in presence of a 250 mT magnetic field. This fully reversible effect increases with progressing magnetization and chain formation. A particle tracking was performed to evaluate the chain formation process and the translation of the particles on a single particle basis [2].

Financial support by DFG (Grant. No. OD18/21) within SPP1681 is gratefully acknowledged.

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Influence of damaged interfaces on poling processes and coupling factors in magnetoelectric composites

Alexander Schlosser (*University of Kassel, Germany*)

09:30

Andreas Ricoeur (*University of Kassel, Germany*)

The efficiency in converting magnetic into electric energy and vice versa makes magnetoelectric (ME) composites promising candidates for many technical applications. The ferroelectric matrix as well as the magnetostrictive inclusions of particle composites and the layers of laminates are mostly ceramics or other brittle materials, thus being prone to cracking. Independent from the kind of composite the transmission of stresses via the interfaces between the constituents plays the key role in the functionality of ME composites. Therefore, the investigation of delamination processes is of great interest for the prediction of durability and coupling factors. In order to investigate delamination processes in ME composites, cohesive elements are being developed and applied in combination with nonlinear ME finite elements described in [1] and [2]. The mechanical behavior of the cohesive zone is classically prescribed by a bilinear traction-separation-law. Magnetic and electric fluxes emanate from evolution laws of magnetic and electric permeabilities, respectively, accounting for micro crack damage in the process zone and electrostatic stresses at the interfaces. Electric and magnetic properties change during damaging processes, being controlled by damage variables, which in turn are determined by the separation between the boundaries. Based on these cohesive elements, possible influence factors on delamination like the geometry of the composites or the ME poling processes are investigated, finally with regard to improving coupling coefficients.

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Nonlinear bilateral caloric-electromechanical couplings in polycrystalline ferroelectrics

Andreas Warkentin (*University of Kassel, Germany*)

09:50

Marius Wingen (*University of Kassel, Germany*)

Stephan Lange (*University of Kassel, Germany*)

Andreas Ricoeur (*University of Kassel, Germany*)

Ferroelectric materials, such as lead zirconate titanate (PZT) or barium titanate (BT) are technically attractive ceramics because of their special properties. They are often used for actuators or sensors in the precision range. The materials are mostly subjected to high frequencies and large electrical loads, which is why insufficient heat dissipation can lead to undesirable temperature developments, so-called self heating.

The letter is due to irreversible domain wall motion and leads to changes in the material properties and sometimes even to phase transformations, whereupon the devices finally are inoperative. In case of insufficient heat dissipation, structural problems due to phase transformations and thermal stresses occur. In low Curie temperature materials, such as barium titanate, even depolarization is possible. Besides the aforementioned nonlinear self-heating, the reversible elasto- and electrocaloric effects demonstrated in experiments [2] have become increasingly important in recent years [4, 5] e.g. with regard to the design of smart cooling devices [5]. In conventional ferroelectric materials, however, large reversible effects occur at high temperatures and are thus often negatively influenced by phase transformation. In [3] a FE model and related simulations are presented with nonlinear ferroelectric materials, forcing into account domain switching induced heating. Although complex thermomechanical boundary value problems can be solved with the FEM, the calculations are very time-consuming. The aim of this work is to extend the so-called condensed method (CM) according to [1] to realize a time-saving and discretization-free possibility to predict the temperature evolution in ferroelectric materials on the basis of a single polycrystalline material point. For this purpose, the CM is extended by the nonlinear bilateral caloric-electromechanical couplings. In addition, a comparison of the results by this work and those of the FEM according to [3] is presented. For verification, the theoretical results from the CM and FEM are compared to the experimental results according to [2].

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S08 | Multiscales and homogenization

Organiser: Benjamin Klusemann (*Leuphana University of Lüneburg, Germany*)
Dennis Kochmann (*ETH Zürich, Switzerland*)

S08.01 | Multiscales and homogenization

Date: February 19, 2019
Room: HS 41

08:30-10:30

A short tour through continuum micromechanics and multiscale modeling of inhomogeneous materials

Helmut J. Böhm (*TU Wien, Austria*)

08:30

A considerable number of continuum approaches to the homogenization and localization analysis ("upscaling" and "downscaling") of inhomogeneous materials have been developed over the past 150 years. They can be grouped into analytical and bounding schemes as well as numerical approaches based on evaluating the responses of specific inhomogeneous volume elements.

The most important of the pertinent modeling strategies are introduced in a short discussion, special emphasis being put on their respective strengths and weaknesses (as seen from the author's perspective as engineer). On this basis, the spotlight is directed, on the one hand, on the interplay between analytical and numerical modeling approaches, predictions for some specific inhomogeneous systems being compared. On the other hand, multiscale modeling strategies are discussed that can be obtained by the sequential application of schemes from the above groups and/or by their incorporation into macroscopic models.

The main emphasis is put on matrix-inclusion composites and throughout the presentation specific issues are highlighted that, from the author's point of view, may merit further detailed study.

A Hashin-Shtrikman type semi-analytical homogenization procedure in multiscale modeling to account for coupled problems

David Jaworek (*RWTH Aachen University, Germany*)
Stephan Wulfinhoff (*Kiel University, Germany*)
Stefanie Reese (*RWTH Aachen University, Germany*)

09:10

Heterogeneous materials are important for a vast amount of applications e.g. in automotive industry or in aerospace. For instance when producing components, it can be desired to use materials with a heterogeneous micro structure in order to achieve specific material properties. The resulting properties are highly dependent on the manufacturing process itself which can involve mechanical or thermal loadings. Therefore it is necessary to properly depict the microstructural material behavior in order to allow for calibration of the manufacturing process and solution of the inverse problem.

Constitutive models can be used to depict the material response in a simplified manner. These simplifications allow for a more flexible use of the model but restrict the applicability to a certain range of use-cases. Thus, it is beneficial to take the materials' microscopic structure into account and couple its behavior to the macroscopical response. As multiscale methods (e.g. FE², FE-FFT) are computationally expensive, semi-analytical homogenization procedures are investigated to account for the transition between different length scales. In this work, the focus lies on a Hashin-Shtrikman type method applied to different processes e.g. elasto-plasticity including phase transformations and also thermo-mechanically coupled processes.

Damage simulation of fibre reinforced composites using mean-field homogenization methods

Peter Lenz (*University of Paderborn, Germany*)

09:30

Rolf Mahnken (*University of Paderborn, Germany*)

A mean-field homogenization framework for constitutive multiscale (meso-macro) modelling including material failure of three distinct linear elastic material phases is presented in this work. Within this framework it is possible to compute the macroscopic mechanical behaviour of fibre reinforced materials based on the constitutive models of the constituents. The three phases are unidirectional fibres surrounded by an interface, which is surrounded by a matrix material. Different mean-field homogenization methods are used to determine the effective properties for example the Mori-Tanaka scheme [4], the self-consistent method [3] and the interaction direct derivative [5], a more recently published method. For homogenization of the three phase composite we use the two-level recursive scheme from [2]. The fibre and interface is regarded as a two-phase composite which, once homogenized, plays the role of a homogeneous inclusion for the matrix material.

A distinction is made between four different failure modes namely matrix failure, fibre failure, matrix-fibre interface failure and a simultaneous failure of the matrix and the fibre called matrix-fibre failure. For matrix failure a critical yield stress is decisive within the matrix. The fibre failure is caused by a high normal stress in direction of the fibre. The shear stress between the fibre and matrix is responsible for the matrix-fibre interface failure. To simulate a crack growth, we use the element deletion method in Abaqus implicit [1]. Representative examples demonstrates the different types of failure and the resulting crack growth in a fibre reinforced material.

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Computational homogenisation of thermo-inelastic composites with an emphasis on weak micro-periodicity

Rolf Berthelsen (*TU Dortmund, Germany*)

09:50

Andreas Menzel (*TU Dortmund, Germany, Lund University, Sweden*)

In this contribution, a thermo-mechanically coupled two-scale finite element framework at finite deformations is considered. The solution of the underlying balance equations, the balance of linear momentum as well as the heat equation, is at both scales carried out in monolithic manner. The scale-bridging between the scales is hereby achieved by application of Hill-Mandel type conditions for the tractions and the heat flux on the boundary of the lower scale. The arising constraints regarding the boundary values of the respective fields, the displacements as well as

the temperature, are fulfilled in a weak sense. Emphasis is laid on the formulation as well as the algorithmic implementation of these boundary conditions which are denoted as "weak boundary conditions" (WK) relating to Larsson et al. [1] who introduced the concept of "weak micro periodicity" for mechanical problems. As a prototype thermo-elastic material model, large deformation thermo-viscoplasticity is considered within this contribution. The performance of the implementation is presented by means of representative numerical examples where the WK boundary conditions are compared against results obtained under application of Dirichlet and Neumann type as well as periodic boundary conditions.

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Homogenization of stiffness and eigenstresses/eigenstrains of matrix-inclusion composites

Nabor Jimenez Segura (*TU Wien - Vienna University of Technology, Austria*) 10:10

Bernhard Pichler (*TU Wien - Vienna University of Technology, Austria*)

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

The Mori-Tanaka scheme is very popular for the homogenization of the elastic stiffness of microheterogeneous composites consisting of one matrix phase and one inclusion phase, see [1]. In addition, the scheme allows for homogenization of eigenstresses/eigenstrains, e.g. in the fields of poroelasticity, thermoelasticity, drying shrinkage, and elastoplasticity [2,3]. Still, the Mori-Tanaka scheme cannot appropriately represent matrix-inclusion composites with non-aligned ellipsoidal inclusion phases, because (i) the respective homogenized stiffness estimate becomes non-symmetrical [4], and (ii) the eigenstrain influence tensors do not satisfy the elastic reciprocal theorem [3]. Recently, an approach for symmetrization of the stiffness tensor was developed [5]. This provides motivation for the present contribution. It introduces a novel extension of the Mori-Tanaka scheme providing eigenstrain influence tensors which are (i) kinematically compatible, in the sense of satisfying the strain average rule, (ii) statistically admissible, in the sense that the stress average rule delivers the same macroscopic stress state as Levin's theorem, and (iii) energetically consistent, in the sense of satisfying the elastic reciprocal theorem.

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S08.02 | Multiscales and homogenization

Date: February 20, 2019

08:30-09:30

Room: HS 41

Molecular dynamics simulation of ultrasonic metal welding of aluminum alloys

Shimaalsadat Mostafavi (*RWTH Aachen University, Germany*)

08:30

Bernd Markert (*RWTH Aachen University, Germany*)

In this study, molecular dynamics simulation of the ultrasonic welding of aluminum alloys is presented. Ultrasonic metal welding is counted as a solid state consolidation of the mating parts, in which the growing interface temperature is far below the melting point of the material and the energy consumption is relatively low compared to the common welding processes such as arc welding. The reciprocating motion of the sonotrode on the mating parts combined with the application of external pressure in the process of ultrasonic welding is the source of temperature rise and strong plastic deformations at the mating interface [1]. This contribution is devoted to study the interactive effect of the process parameters on the interface temperature, deformation process of the mating parts and the diffusion behavior of the interface atoms.

[1] S. Mostafavi, DF. Hesser, B. Markert, 2018. Effect of process parameters on the interface temperature in ultrasonic aluminum wire bonding. *J. Manuf. Process.*, P. 336-344.

Virtual testing of additively manufactured grid structures

Ulrike Gebhardt (*TU Dresden, Germany*)

08:50

Roland Gärtner (*Leichtbauzentrum Sachsen GmbH, Germany*)

Stefan Holtzhausen (*TU Dresden, Germany*)

Markus Kästner (*TU Dresden, Germany*)

Additive Manufacturing is a flexible technology with very high potential to produce lightweight structures. Selective Laser Melting (SLM) enables the production of grid structures from AlSi10Mg metal powder. These grid structures can be used to build lightweight components with high load carrying capacity.

In this contribution, an experimental and virtual multiscale approach to material characterization is presented to predict the effective mechanical behaviour of additively manufactured grid structures.

To characterise the base material, tensile tests are performed to determine basic material parameters after manufacturing. These are input for a computational homogenization. A unit cell representing the minimal repeating geometry of the grid structure is used to simulate the local stresses at the joints and to obtain effective values for material parameters. To validate the modelling approach, larger specimens for shear, torsion, tensile and pressure tests are manufactured. The experimental results are compared to virtual experiments using a homogeneous material with effective properties from the unit cell simulation as well as a detailed model resolving the exact geometry of the grid structure.

The mechanical behaviour of additively manufactured components strongly depends on the process parameters used to build those components. E.g. the macroscopic additively manufactured grid structures show imperfections such as additional material at the bars or pores within the bulk material. Those imperfections are quantified and a first numerical analysis of their influence on the overall behaviour is presented.

The authors would also like to acknowledge the support of Dr.-Ing. Matthias Berner (Leichtbauzentrum Sachsen GmbH) and Dr. Uta Kühn (Leibniz Institute for Solid State and Materials Research Dresden).

Laser shock peening: modelling across scales

Benjamin Klusemann (*Leuphana University of Lüneburg, Germany, Helmholtz-Zentrum Geesthacht, Germany*) 09:10
Sören Keller (*Helmholtz-Zentrum Geesthacht, Germany*)
Vasily Pozdnyakov (*Leuphana University of Lüneburg, Germany*)
Jens Oberrath (*Leuphana University of Lüneburg, Germany*)
Nikolai Kashaev (*Helmholtz-Zentrum Geesthacht, Germany*)

Laser shock peening is a surface modification technique to improve the fatigue performance of metallic structures by inducing compressive residual stresses for mitigation of crack growth. A pulsed laser vaporizes the first layer of the component and turns the solid material into plasma. Thermal expansion of the plasma in the confining medium initiates high pressure shock waves propagating into the material. Residual stresses are the result of local plastic deformations caused by the pressure waves. The process is highly nonlinear involving a high number of process parameters, short time events and extreme values of physical quantities. Aiming at deeper understanding of the process, a modeling approach across different scales is proposed. Starting with a laser induced plasma shock wave simulation, a global model for determining the shock pressure depending on the laser parameters is employed. The results of the shock pressure distribution over time are used in a subsequent LSP process simulation, to predict the resulting residual stress profile and plastic deformation within the material. Subsequently a transfer approach based on the eigenstrain-method to include the plastic deformations in a finite element model of a C(T)-specimen which is used to predict the residual stresses and the stress concentration for different external loads, is proposed. Empirical FCP-equations are used to predict the FCP rate. Comparison and validation of the numerical results on basis of experimental results will be presented.

S08.03 | Multiscales and homogenization

Date: February 20, 2019 14:00-16:00
Room: HS 41

Modern non-linear solution techniques in FFT-based computational micromechanics

Matti Schneider (*Karlsruhe Institute for Technology (KIT), Germany*) 14:00

The FFT-based homogenization technique, originally introduced by Moulinec and Suquet, has become the major workhorse for the computational homogenization of heterogeneous materials characterized by a complex microstructure, often characterized by 3D imaging techniques. As voxels serve as finite elements, the non-linear solution techniques need to be both memory-efficient and extremely robust. In this contribution, we give an overview of recent improvements in these solution techniques, including fast gradient methods, polarization techniques and quasi-Newton solvers.

A model order reduction method for finite strain FFT solvers using a compressed sensing technique

Christian Gierden (*RWTH Aachen University, Germany*) 14:40
Julian Kochmann (*RWTH Aachen University, Germany*)
Kiran Manjunath (*RWTH Aachen University, Germany*)
Bob Svendsen (*Max-Planck-Institut für Eisenforschung GmbH, Germany*)
Stefanie Reese (*RWTH Aachen University, Germany*)

Recently, FE-FFT based methods (e.g., Kochmann et al., 2016) have been developed which seem to be more efficient than FE² methods. Within this context, we present a novel model order reduction technique for FFT solvers to reduce the computational costs for the FFT simulation scheme. The underlying method is based on a compressed sensing technique (e.g., Candes et al., 2006) which is used to reconstruct a highly incomplete data set. Concerning FFT solvers, a reduced set of frequencies may be used to calculate a reduced numerical solution of the Lippmann-Schwinger equation. The aforementioned reduced set of frequencies is determined offline and consists predominantly of low frequencies. In a post-processing step the compressed sensing technique is employed to reconstruct highly resolved micromechanical fields (Kochmann et al., 2018). To solve the boundary value problem, classical fixed-point iterations are performed. Compared to the unreduced solution, a significant speed-up in CPU times at a negligibly small loss of accuracy in the overall constitutive response is observed. The developed reduction technique does not require any time-consuming offline computations, e.g. for the generation of snapshots, is not restricted to any kinematic or constitutive assumptions and its implementation is straightforward. Elastic composites are investigated in a finite strain setting as representative simulation examples.

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Kochmann, J., Manjunatha, K., Gierden, C., Wulfinghoff, S., Svendsen, B., Reese, S., 2018. A simple and flexible model order reduction method for FFT-based homogenization problems using a sparse sampling technique. Submitted for publication.

Kochmann, J., Wulfinghoff, S., Reese, S., Mianroodi, J. R., Svendsen, B., 2016. Two-scale FE-FFT- and phase-field-based computational modeling of bulk microstructural evolution and macroscopic material behavior. *Computer Methods in Applied Mechanics and Engineering* 305, 89-110.

An explicit solution of implicit single crystal small-strain viscoplasticity and its use in FFT-based micromechanics

Daniel Wicht (*Karlsruhe Institute of Technology (KIT), Germany*)

15:00

Matti Schneider (*Karlsruhe Institute of Technology (KIT), Germany*)

Thomas Böhlke (*Karlsruhe Institute of Technology (KIT), Germany*)

Computational homogenization schemes based on the fast Fourier transform [1] enable studying the micromechanical behavior of polycrystalline microstructures with complex morphology [2]. In the conventional strain-based setting, evaluating the single crystal elasto-viscoplastic constitutive law involves solving a non-linear system of equations. The latter is ill-conditioned, in particular for a large viscoplastic exponent, and its solution dominates the overall runtime. Evaluating the inverse material law is much less costly in the small-strain context, because the flow rule is an explicit function of the stress, cf., e.g., Lebensohn et al. [2]. We investigate the FFT-based simulation of polycrystalline materials based on the stress-based dual formulation of the Lippmann-Schwinger equation [3] in terms of performance and convergence behavior for polycrystalline fibrous microstructures of directionally solidified eutectics [4].

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Informed training with increasing fidelity: modeling dynamic recrystallization from Taylor to FFT-based Field Monte Carlo Potts

Abbas Davud Tutcuoglu (*ETH Zurich, Switzerland, Caltech, USA*)

15:20

Dennis M. Kochmann (*ETH Zurich, Switzerland, Caltech, USA*)

Discontinuous dynamic recrystallization (DDRX) describes the process of texture and microstructure evolution through nucleation and grain boundary migration parallel to deformation. Observed mainly in low-to-medium stacking fault energy metals, this inherently atomistic process has been subjected to numerous modeling attempts at the continuum scale. Following fully homogenized models such as the Johnson-Mehl-Avrami-Kolmogorov (JMAK) relation describing the evolution of a recrystallized volume fraction, Monte-Carlo Potts, cellular automata, vortex methods, and similar approaches shifted the modeling to a representative volume element (RVE) on the mesoscale to include the spatial, curvature-driven component of nucleation and migration. Subsequent work on the underlying material and particularly plasticity models allowed to relax the assumptions made with regards to DDRX modeling, including a dependence of nucleation on the locally stored inelastic strain energy density, extensions to finite deformations as well as the inclusion of anisotropic inelasticity.

In previous work, we have successfully combined all these properties including the capturing of inhomogeneous deformation within grains in a computationally feasible way thanks to an FFT-based Field Monte Carlo Potts (FMCP) method [1,2]. Having showcased the full capabilities of this FCMP model using a highly anisotropic magnesium model including slip-twin-interactions, we discuss the additional virtue of high-fidelity vertical homogenization approaches such as the one described here based on uniaxial compression experiments conducted on copper [3]. Alongside the comparison of accuracy and computational expense, we further propose a training technique, in which the computationally inexpensive fitting of homogenized approaches such as the Taylor model can be used to inform fully resolved simulations of DDRX on the mesoscale using FMCP.

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Preconditioning of the spectral Fourier method for homogenization of periodic media

Martin Ladecký (*Czech Technical University in Prague, Czech Republic*)

15:40

Ivana Pultarová (*Czech Technical University in Prague, Czech Republic*)

Jan Zeman (*Czech Technical University in Prague, Czech Republic*)

We consider a homogenization problem over a rectangular domain with periodic boundary conditions. For numerical solution, we use the Galerkin or collocation method employing the spectral Fourier basis. The purpose of our presentation is to show that the matrix of the associated system of linear equations can be preconditioned by a matrix arising from a problem corresponding to the data of the original homogenization problem which are simplified in a certain manner.

The matrix associated to this simplified problem is sparse (diagonal or multi-diagonal). This kind of preconditioning can avoid influence of anisotropy and of some oscillatory components of the data. We introduce sharp guaranteed theoretical upper bound to the condition number of the preconditioned problem. Some relevant numerical experiments are presented.

S08.04 | Multiscales and homogenization

Date: February 20, 2019
Room: HS 41

16:30-18:30

Computational finite strain homogenization: reduced basis methods and beyond

Oliver Kunc (*University of Stuttgart, Germany*)
Felix Fritzen (*University of Stuttgart, Germany*)

16:30

Mechanical homogenization problems emerge from both industrial and academic contexts. Usually, the FE² method serves as a benchmark problem since it can reach any desired accuracy. However, it is also known to come along with high computational burdens. This work contributes to the field of homogenization methods with emphasis on efficiency. Reduced basis methods are investigated for their suitability for hyperelastic homogenization problems. The task is to find a kinematic quantity that is suitable for efficient reduction. First results are already promising, and additional theoretical considerations could possibly lead to further speed-ups in the online phase. Considering the offline phase, a high-dimensional sampling strategy is proposed. It compromises completeness and sparsity, crucial for efficiency. Numerical results of realistic two-scale simulations are anticipated.

An artificial neural network based solution scheme to periodic homogenization

Felix Selim Goekuezuem (*University of Stuttgart, Germany*)
Lu Trong Khiem Nguyen (*University of Stuttgart, Germany*)
Marc-André Keip (*University of Stuttgart, Germany*)

17:10

Motivated by the enormous research progress on the field of machine learning [1,2], the present contribution presents a solution algorithm for periodic homogenization problems based on an artificial neural network (ANN) discretization. Here, we follow closely the idea of Lagaris et al. [3], who suggested the use of ANN-based trial functions that by construction fulfill the given boundary conditions. Regarding the homogenization framework, we assume that the macroscopic response of a material is governed by a periodic boundary value problem of a representative volume element (RVE) on the microscale [4]. We thus construct trial functions through singlelayer and multilayer ANNs that fulfill a priori the periodic boundary conditions of the microstructure problem. In order to find the physical equilibrium, a global energy potential serves as an objective function, which by construction of the trial function can be optimized without constraints.

In this work, we will restrict ourselves to the case of electrostatic boundary value problems driven by the electric potential as scalar-valued independent field. Aim of the new approach is to reduce the number of unknowns, as we assume that the ANNs are able to fit complicated functions with a comparably little number of internal parameters. We investigate the viability of the scheme on the basis of one, two and three dimensional microstructure problems. As an optimizer, the L-BFGS algorithm [5] is applied and its convergence behavior numerically evaluated. Further, continuous and discontinuous approaches for constructing the trial function are discussed and compared to finite-element (FE) method and fast Fourier transform (FFT) based simulations.

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Application of a machine learning and data mining approach to determine relationships in materials science

Frederic E. Bock (*Helmholtz-Zentrum Geesthacht, Germany*)

17:30

Norbert Huber (*Helmholtz-Zentrum Geesthacht, Germany*)

Benjamin Klusemann (*Helmholtz-Zentrum Geesthacht, Germany, Leuphana University of Lüneburg, Germany*)

The application of machine and statistical learning approaches in materials science represents a powerful instrument for accelerating the development of novel materials, processes and techniques. One of the overall challenges for materials scientists and engineers is the identification of relationships along the process-structure-property chain, which usually involves the bridging of numerous scales that differ considerably in magnitude. Data mining and machine learning can be performed with high-throughput of experimentally and numerically produced data sets to generate an output of highly efficient and reliant knowledge for materials characterization and optimization across various scales. Ultimately, the specific approach and its suitable applicability highly depends on the involved use-cases, processes, materials, spatial and temporal scales, data-types, formats, as well as required computational costs and anticipated understanding. A concrete application of a machine learning and data mining approach to determine a particular process-microstructure-property relation will be presented.

Adaptivity in reduce order computational homogenization using neural networks

Mauricio Fernández (*University of Stuttgart, Germany*)

17:50

Felix Fritzen (*University of Stuttgart, Germany*)

Multiscale simulations for large scale structures incorporating constitutive behavior of the microscale can be approached only to a limited extend by computational approaches as the FE² ansatz. This is due to the increasing computational expenses and time of the finite element computations at the microscale required at every Gauss point of the macroscale. In order to accelerate the microscopic computations, the present work combines the efficiency of a reduced order model (ROM) and the properties of a neural network (NN). A ROM based on a reduced basis is used to obtain a physically motivated surrogate. The ROM is used to generate a rich data set and so provide rapid initial guesses for additional FE simulations. The NN is trained with the machine learning library TensorFlow based on the gathered FE and ROM simulation data in order to calibrate error estimates for different dimensions of reduced bases. For prescribed accuracy, the NN returns an estimate for the minimum dimension of the reduced basis, such that online ROM computations can be carried out adaptively at lower computational expense based on our a priori error estimate. Examples for pseudo-plasticity are presented.

Computational runtime acceleration within TPM² environment

Florian Bartel (*TU Dortmund University, Germany*)

18:10

Tim Ricken (*University of Stuttgart, Germany*)

Jörg Schröder (*University of Duisburg-Essen, Germany*)

Joachim Bluhm (*University of Duisburg-Essen, Germany*)

Thinking about the description of porous materials, e.g. metal foam, human tissue, plants or soils, we always have to take into account a global design composed of various substructures with different characteristics on a lower level. Examples of such substructures are pores which can be saturated with fluids or gases, fibers with different orientations or cells which can be influenced by chemical reactions. For the theoretical description of the behavior, enhanced continuum mechanical models give promising approaches. Up to now, due to the high complexity, it has not been possible to simulate these systems with a continuous discretization up to the microstructural level. Hence, it is necessary to think about techniques which simplify the model but still consider the essential characteristics.

Future applications will have the opportunity to consider the discrete microstructure of materials. For example, the topology can be received by CT-scanning technology and the received image data can be transferred to a finite element mesh. Furthermore, Representative Volume Elements (RVEs) can be designed based on the image data of the internal structure. Therefore, we are developing the TPM²-Method which is considered as the Theory of Porous Media (TPM), see [1], embedded into the two-scale, first-order homogenization scheme of the FE²-Method, cf. [2]. This contribution will present a two-scale homogenization approach for fluid saturated porous media with a reduced two-phase material model, which covers the behavior of large poro-elastic deformation. The main aspects of theoretical derivation for the weak form, the lower level boundary conditions under consideration of the Hill-Mandel homogeneity condition and the averaged macroscopic tangent moduli will be discussed and a numerical example will be shown. However, solving a 3-dimensional, nonlinear, coupled and time dependent problem in a FE² environment is extremely computational expensive. Therefore, a parallel solution strategy is absolutely essential. Remarks on the investigation of High Performance Computation will be given in this context.

Besides, machine learning technologies are promising for an impressive improvement of runtime. Hereby one has to face approximation inaccuracy, however errors are small for engineering applications. Hence, we are applying Artificial Neural Networks (ANN). Conceptual ideas will be pointed out.

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S08.05 | Multiscales and homogenization

Date: February 21, 2019

08:30-10:30

Room: HS 41

Simulation of dual-phase steel using the finite cell method and voxel-based microstructure data

Yannick Francis Fangye (*Ruhr University Bochum, Germany*)

08:30

Niklas Miska (*Ruhr University Bochum, Germany*)

Daniel Balzani (*Ruhr University Bochum, Germany*)

Dual-phase (DP) steels are frequently used materials for many engineering applications due to their attractive mechanical properties such as high ductility and high ultimate tensile strength. These properties are directly dependent on the interactions of the individual microscopic constituents, namely ferrite and martensite. To quantify their effective macroscopic response in the framework of computational homogenization, the morphology of their microstructure needs to be taken into account in modeling and simulation. A suitable finite element discretization of the microstructure can be constructed by applying the method proposed in [1]. There, the microstructure of dual-phase steel is measured using three-dimensional EBSD and associated voxel data is obtained which distinguishes between the ferrite and the martensite. Subsequently, a smooth morphology description is constructed and a conforming finite element mesh is generated. This method, however, is comparatively expensive since the construction of the smooth morphology requires significant effort and the resulting finite element mesh may also contain many degrees of freedom. An alternative is to apply the finite cell method [2, 3], where a regular mesh is considered and the microscopic material decomposition is included in terms of subcells used for the integration. Especially for microstructures given by voxel-based data the step to construct a smooth morphology can thereby be avoided. In this presentation it is shown that a significantly improved efficiency with respect to multiscale simulations of DP steel can be realized by using the finite cell method. Furthermore, an adapted subcell decomposition method is proposed which directly exploits the nature of voxel-based data. This method will be compared with the classically applied octree method in terms of efficiency and accuracy in finite element simulations representing the experimental response of DP steel.

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Goal-oriented adaptivity on mean-field and full-field homogenization methods considering hierarchical unit cells

Xiaozhe Ju (*University of Paderborn, Germany*)

08:50

Rolf Mahnken (*University of Paderborn, Germany*)

Homogenization methods are drawing increasing attention for simulation of heterogeneous materials like composites. For balancing the accuracy and the numerical efficiency of such simulation, we deal with both model and discretization errors of the finite element method (FEM) on a macro scale. Within a framework of goal-oriented adaptivity [1-4], linear elastic heterogeneous materials, for which first order homogenization schemes apply, are handled. In doing so, particular attention is paid to establish a novel model hierarchy. This model hierarchy contains mean-field homogenization methods as a basic model, which can be enhanced by a full-field approximation, where a unit cell problem is solved via the FEM under an a priori chosen boundary condition. For a further stage of the model hierarchy, we consider hierarchical unit cells within the frame of the FEM towards an adaptive selection of unit cell size. By means of several numerical examples, we illustrate the effectiveness of the proposed adaptive approach.

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Homogenization of cementitious materials: stiffness, creep, strength

Bernhard Pichler (*TU Wien - Vienna University of Technology, Austria*)

09:10

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

Multiscale modeling of heterogeneous materials consists of resolving their microstructure down to scales at which material constituents are found that can be described based on material constants rather than on evolving material parameters. Concrete is a matrix-inclusion composite, with aggregates and sand embedded in a cement paste matrix. The properties of cement paste are not constant. Instead, they are a function of the composition and the maturity of the material, i.e. they depend on the initial water-to-cement mass ratio and the degree of hydration. From the viewpoint of multiscale modeling, cement paste is a matrix-inclusion composite, with residual cement grains embedded in a hydrate foam matrix. The hydrate foam, in turn, is a highly randomized arrangement of partially saturated capillary pores and needle-shaped hydration products. In the present contribution, it is shown that material constants assigned to the microscopic hydration products, allow for predicting the hydration-driven evolutions of stiffness, creep, and strength of cementitious materials [1-12]. These models were developed at the Institute for Mechanics of Materials and Structures at TU Wien - Vienna University of Technology. It can be shown that the behavior of hydration products is governed by simple physical laws. The latter translate, because of microstructural interactions with the other constituents, into the complex macroscopic behavior of cementitious materials observed in macroscopic material testing.

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Multiscale analysis of heterogeneous materials in boundary representation

Maximilian Praster (*RWTH Aachen, Germany*)

09:30

Rainer Reichel (*RWTH Aachen, Germany*)

Sven Klinkel (*RWTH Aachen, Germany*)

This paper deals with a numerical method for modeling heterogeneous materials with nonlinear behavior. Many novel high-performance materials consist of different components. In the frame of nonlinear behavior the resulting macroscopic material properties cannot be determined without great experimental effort. In order to simulate the nonlinear material behavior, a nested finite element method (FE²) is used. An accompanying homogenization is performed for each load step. The material behavior is determined from the represented volume element (RVE) on the heterogeneous micro structure. The present approach is dealing with a discretization method of the heterogeneous structure. It based on the geometrical data of the interface boundary of the different constituents. A quad-tree algorithm, in combination with a trimming algorithm is used for the mesh generation. Based on the geometrical data it yields an initial mesh for the analysis. Within the algorithm a staircase approximation of voids or inclusions is circumvented. However, the resulting mesh yields polygonal elements with an arbitrary number of nodes on the element boundary. To this end a novel polygonal element formulation is provided. It is based on the scaled boundary finite element method (SBFEM). The basic idea is to scale the boundary representation in relation to a scaling center. In contrast to SBFEM the present method makes us of an approximation of the displacement response in scaling direction. This enables the analysis of geometrical and material-related nonlinear problems in solid mechanics. The interpolation at the boundary in circumferential direction is independent of the interpolation in scaling direction. This allows for novel refinement strategies, where e.g. p-refinement is only applied for the interior element domain. The internal degrees of freedom are eliminated by static condensation. It leads to an element formulation with an arbitrary number of nodes at the element boundary. Thus, the present element is perfectly suited for a quad-tree meshing algorithm of the RVE. Its hierarchical, tree-like data structure makes it very useful for adaptive mesh refinements of complex geometries and regions with localized gradients. The classical hanging-nodes problem for standard elements is omitted by the present element formulation. Some numerical examples show the capability of the formulation with respect to the numerical homogenization of heterogeneous materials.

Influence of specific core reinforcement designs on the stiffness behaviour of hybrid core sandwich panels

Isabella C. Skrna-Jakl (*TU Wien, Austria*)

09:50

Dieter H. Pahr (*TU Wien, Austria, Karl Landsteiner Private University of Health Sciences, Austria*)

A well-known disadvantage of sandwich structures is their very low out-of-plane shear stiffness, which must not be neglected in the design phase. Hybrid core sandwich structures, consisting of a foam core reinforced with thin composite beams, overcome this issue and thus represent a very efficient lightweight construction concept. Current and future application areas of these kinds of structures are, in addition to aerospace structures, industrial fields such as wind energy, transportation systems, ship building and roof constructions.

The investigated hybrid core exhibits - due to its anisotropic 1D reinforcements oriented at 45° - an improved out-of-plane stiffness behaviour. Purpose of the present study is to numerically investigate the influence of specific core reinforcement designs on the out-of-plane as well as the inplane stiffness behaviour of hybrid core sandwich panels, taking into account the increase in weight due to the built-in stiffeners. Finite Element unit cell analyses are performed employing the homogenization software MEDTOOL [www.dr-pahr.at].

3D-solid FE-models are used to study the changes of the engineering constants due the following parameter variations:

- change of the reinforcement material from UD-composite to pure matrix material,
- the presence of matrix joints in the crossing region of adjacent stiffeners,
- interpenetration of stiffeners at the crossing point, and
- omission of the foam core.

The results show a significantly different behaviour for inplane and out-of-plane responses. On the one hand, the specific inplane engineering constants may decrease by up to 17%, in comparison to the data obtained from unit cell analyses of the unstiffened foam core sandwich, depending on the parameters selected. The reason for the decrease is that the inplane stiffnesses are mainly determined by the behaviour of the face layers and the core stiffeners cause predominantly an increase in weight. On the other hand the results show that the specific values of the out-of-plane pressure and shear stiffnesses can be increased up to 16-fold and 60-fold, respectively, compared to the corresponding results of a foam core sandwich without stiffeners. The distinct increase of these values is due to the orientation of the beams in the direction of principal stresses.

In addition FE-analyses of standardized sandwich compression tests are performed, employing “structural” rather than periodicity boundary conditions. The comparison of the effective out-of-plane engineering constants obtained by the numerical test and unit cell analyses are used to evaluate experimental results.

Laminate-based modeling of semicrystalline polymers

Johannes Ruck (*Karlsruhe Institute of Technologie, Germany*)

10:10

Philipp Kloza (*Karlsruhe Institute of Technologie, Germany*)

Sebastian Gajek (*Karlsruhe Institute of Technologie, Germany*)

Thomas Böhlke (*Karlsruhe Institute of Technologie, Germany*)

Semicrystalline polymers such as, e.g., polyethylene or polyethylene terephthalate, are omnipresent in engineering applications. These polymers exhibit spatially distinct regions of amorphous and crystalline phases. Due to differing thermo-mechanical material behavior of each phase, the material’s microstructure has a pronounced influence on the effective properties of the material. The microstructure is mainly determined by the thermo-mechanical manufacturing process. Additionally, temperature and loading history can influence phase composition, as well, such that modeling phase and glass transitions need to take these aspects into account.

The work at hand covers the phase and glass transition behavior of semicrystalline polymers based on a micromechanical model. To this end, the microstructure is idealized as a three-phase, rank-one laminate model in order to model first- and second-order phase transitions

subject to small strains. The laminate model is set up on previous works [1] and enables the consideration of the polymer microstructure as well as stress and strain localization. The three-phase laminate model consists of a crystalline phase, a rigid amorphous phase and a mobile amorphous phase [2]. Additionally, glass transition effects are taken into account employing a phenomenological approach from the literature [1]. Using a thermodynamically consistent continuum model, the phase transition can be described by the movement of singular surface boundaries inside the laminate structure. As a first approximation, the shear viscosity is not considered and the material behavior is assumed to be isotropic. The phase transition in the thermodynamic equilibrium is considered as a process that minimizes the free Helmholtz energy of the laminate with respect to the volume fractions, the orientation of the phase boundaries as well as the internal variable describing glass transition effects. In order to simulate the interface kinetics in non-equilibrium cases, phenomenological evolution equations are taken from the literature [1] to describe non-equilibrium phase and glass transitions.

Numerical simulations demonstrate that the three-phase laminate model is able to qualitatively represent temperature and deformation-history dependent crystallization under consideration of glass transition effects.

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S08.06 | Multiscales and homogenization

Date: February 21, 2019

14:00-16:00

Room: HS 41

Virtual elements for the homogenization of polycrystalline materials: evidence of locking-free responses with strong anisotropies

Michele Marino (*Leibniz Universität Hannover, Germany*)

14:00

Blaž Hudobivnik (*Leibniz Universität Hannover, Germany*)

Peter Wriggers (*Leibniz Universität Hannover, Germany*)

The computational homogenization of polycrystalline materials is associated with requests of flexibility with regards to mesh generation and element shapes. From the computational point of view, this might couple with the challenge of treating strong and random anisotropies. In this framework, the virtual element method (VEM) has been recently introduced [1] and it has been attracting attention in the framework of advanced modeling techniques for anisotropic material behavior [2] and homogenization of composite materials [3]. This method permits the use of polygonal/polyhedral elements which might perfectly fit grain geometries in the polycrystalline material. Moreover, the VEM rationale allows also to employ advanced homogenization approaches. These advantages are paid in terms of a rank-deficiency of the energy functional due to the projection of the primary variable on a polynomial space. Hence, a stabilization term is conveniently introduced [4].

This work analyzes the performance of a VEM-based computational homogenization approach of polycrystalline materials with respect to FEM-based approaches. Applications are conducted both in linear (infinitesimal) elasticity and in nonlinear (finite) elasticity. For the latter, by the use of the representation theorem for tensor functions, suitable structural tensors allow to define a minimal basis of tensor invariants for the definition of constitutive equations under the respect of assigned material symmetries. Obtained results show the outperformance of a VEM approach with respect to a standard FEM one on the predicted value of homogenized quantities. The coarse mesh permitted by the VEM rationale (where each grain represents one

element) allows to maintain a low computational cost with a high accuracy. From a general computational point of view, analyses on stress distributions allow to show that VEM elements do not show locking due to strong anisotropies. This locking-free response is then competitive with constrained variational formulations which can be introduced in order to mitigate element locking induced by anisotropies.

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The explicit jump discretization with Lippmann-Schwinger solvers for thermal computational homogenization problems

Christian Dorn (*Karlsruhe Institute of Technology (KIT), Germany*)

14:20

Matti Schneider (*Karlsruhe Institute of Technology (KIT), Germany, Fraunhofer Institute for Industrial Mathematics ITWM, Germany*)

We present a Lippmann-Schwinger equation for the explicit jump discretization of thermal computational homogenization. Our solution scheme is based on the fast Fourier transform and thus fast and memory-efficient. Originally Wiegmann and Zemtis introduced the explicit jump discretization as the discrete equivalent of a boundary integral equation for the jump in the temperature gradient. In this boundary integral formulation the resulting system is not symmetric positive definite and hence solved with BiCGSTAB. We reformulate the explicit jump discretization using harmonically averaged thermal conductivities and obtain a symmetric positive definite system. Thus, a Lippmann-Schwinger formulation is possible. In contrast to Fourier and finite difference based discretization methods the explicit jump discretization does not exhibit ringing and checkerboarding artifacts. We demonstrate our improvements by numerical experiments involving the basic scheme, the conjugate gradient method and the polarization-based scheme of Eyre-Milton, comparing the explicit jump discretization to the Fourier discretization of Moulinec-Suquet and the rotated staggered grid of Willot.

Investigation on numerical solution schemes for describing phase transformations by the Kampmann-Wagner numerical model

Jan Herrnring (*Zentrum für Material- und Küstenforschung GmbH, Germany*)

14:40

Benjamin Klusemann (*Zentrum für Material- und Küstenforschung GmbH, Germany, Leuphana University of Lüneburg, Germany*)

Thermo-mechanical processes are of high interest for materials research and industrial applications. Phase transformations occur frequently in heat treatments, joining processes as well as additive manufacturing and have a significant influence on the mechanical properties in the solid and liquid state. One established method for modelling nucleation and growth of phases is the Kampmann-Wagner-numerical (KWN) model. This approach is especially suitable for multiscale process simulations and has been used recently by the authors for the simulation of residual stress fields via a multiscale approach. However, depending on the degree of model complexity the computational effort increases significantly because of the rising amount of phases as well as the effort for solving the evolution equations. Therefore, the simulation of several phases

requires the storage of several fine discretized phase distributions in every integration point. The solution of the conservation law is often realized by schemes of low convergence rate. For the application of the KWN model in a multiscale simulation environment, the usage of numerical solution schemes with higher convergence rate for numerical cost reduction as well as numerical error control is of high interest. Therefore, the authors apply different numerical integration schemes to reduce the numerical effort for the KWN model.

Isogeometric multiscale modeling with Galerkin and collocation methods

Milad Amin Ghaziani (*Technical University of Braunschweig, Germany*)

15:00

Josef Kiendl (*Norwegian University of Science and Technology, Norway*)

Laura De Lorenzis (*Technical University of Braunschweig, Germany*)

Computational homogenization for a two-scale boundary value problem (BVP) in the framework of the finite element method (FE2) is well established but is known to be computationally demanding. In this contribution, we apply computational homogenization by means of isogeometric analysis (IGA) and denote this method as IGA2. Its efficient implementation and the development of computationally efficient integration rules are main issues.

With the aim to reduce the cost of integration for IGA, isogeometric collocation (IGA-C) has been recently introduced. The main idea is that the higher continuity of the basis functions, enables the direct discretization of the strong form of the governing equations. IGA-C requires only one evaluation point per degree of freedom, regardless of the polynomial degree of the basis functions.

In this work we test IGA-C for computational homogenization with the goal of solving a two-scale BVP more efficiently. As a first step, we utilize IGA-C at the macro scale. The number of macroscopic evaluation points is dramatically reduced and a substantial gain in efficiency is obtained over the IGA2 and FE2 techniques. Moreover, employing IGA-C in the micro BVP leads to an additional gain in computational efficiency, as a result of the decreased number of evaluation points at both scales. The different methods and their combinations across the two scales are investigated and compared in terms of efficiency and robustness.

Diffuse modelling of weak discontinuities

Paul Hennig (*TU Dresden, Germany*)

15:20

Dominik Schillinger (*University of Minnesota, USA*)

Markus Käßtner (*TU Dresden, Germany*)

In the numerical analysis of heterogeneous materials, weak discontinuities arise in the field variables due to rapidly changing mechanical properties at material interfaces.

Details about the local topology of heterogeneous microstructures are typically taken from imaging methods or are given in terms of random distributions. To avoid costly meshing processes, embedded domain methods can be used. They embed the physical domain directly into a regular background mesh, that is used for computation. While good convergence rates can be achieved for homogeneous materials, stress oscillations occur in the heterogeneous case because weak discontinuities are modeled in terms of a continuous basis.

For that reason, we propose two approaches that are based on a regularization of the sharp material interface. In the first approach a static phase field is introduced that smears the material interface over a given length scale. To define the material properties in the transition region, homogenization assumptions are used that fulfill the balance of linear momentum at the interface and kinematic compatibility. In the second approach, we directly apply this homogenization onto the interface element. To further increase the efficiency of the methods, adaptive local h-refinement is applied towards the interface.

Both approaches are compared in terms of convergence of the energy towards the sharp interface limit which is investigated in several benchmark problems. It will be shown that the choice of the homogenization approach as well as the definition of the static phase-field are of high importance, because they even influence the quality of the solution in the domain far away from the interface. It is demonstrated that optimal convergence can be obtained in the far field under special circumstances.

Implementing a microstructure model of rubber with self-organization into a FEM Software

Erik Oelsch (*Chemnitz University of Technology, Germany*)

15:40

Hans Wulf (*Chemnitz University of Technology, Germany*)

Jörn Ihlemann (*Chemnitz University of Technology, Germany*)

Experimental investigation of filled rubber reveals several complex properties like hysteresis, permanent set, Mullins-effect. The connection of these properties to the microstructure is still unclear. The theory of Self-Organizing Linkage Patterns (SOLP) by Ihlemann is an approach that relies crucially on deviations from average distributions. Specifically, it states that deformed rubber develops a pattern based on physical linkages, which is characterized by regions of high and low linkage density. On this basis, all complex material properties can be explained as result of an adaption of the linkage pattern to the applied deformation. The theory is verified by a simulation program, which uses a very abstract model of the molecular structure of filled rubber. With this C++ program it is possible to generate stress-strain curves according to a loading schedule. The model is generated randomly, which has a huge influence on the results. Therefore a FEM software is used to smooth these curves with a 2D model that mixes serial and parallel connections of single SOLP systems. Each Gaussian point has a SOLP system with different starting conditions. The model is highly discontinuous because of the constant reorganization, which leads to rough numerical properties for a FEM software. An interface was created to implement this complex model with high computation times into Abaqus. With the explicit FEM method it is possible to use this microstructure model for 2D simulations.

S08.07 | Multiscales and homogenization

Date: February 21, 2019

14:00-16:00

Room: SR 03

Finite element simulations and nonlinear homogenization of fibre reinforced elastomer composite

Tilen Ceglar (*TU Wien, Austria*)

14:00

Heinz E. Pettermann (*TU Wien, Austria*)

Fibre reinforced elastomers (FREs) made of continuous fibres embedded in a hyperelastic matrix exhibit highly anisotropic properties. The fibres provide excellent stiffness and strength in the fibre direction while the matrix allows considerable deformations and large failure strain perpendicular to the fibres. Such materials are widely used in tyres, power transmission belts and are also present in biological tissues.

The pronounced anisotropic nature of FREs and the strong influence of shape, size and arrangement of fibres make it difficult to successfully employ analytical homogenization strategies. Most of the available anisotropic hyperelastic material models for the homogenized behaviour are purely phenomenological and are typically subject to non-trivial material parameter fitting. However, they are essential for structural analysis of components made from FREs.

In the present work, the effective response of aligned continuous glass fibres randomly embedded in a silicon rubber matrix is predicted for selected load cases by means of nonlinear Finite Element Method (FEM) unit cell simulations. The effective response is studied in the finite strain regime with respect to different fibre arrangements and sizes of unit cells.

Besides the nonlinear homogenization by the unit cell simulations, phenomenological anisotropic hyperelastic material models are employed to approximate the effective behaviour of FREs. Most of their material parameters can be calibrated by consideration of the linearised initial behaviour. For the anisotropic hyperelastic material models considered in this work, the fitting is minimised to adjust a single parameter, which influences the nonlinear progression in the response.

Unit cells with periodic boundary conditions are simulated in transverse, axial and combined load cases. The effective response of unit cells under each load case are compared to the single element simulations utilizing the calibrated phenomenological material models. Good agreement between the results is found for moderate stretches and fibre volume fractions of 20%-30%.

Acknowledgement:

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Magneto-electric product properties of multiferroic composites

Matthias Labusch (*University Duisburg-Essen, Germany*)

14:20

Jörg Schröder (*University Duisburg-Essen, Germany*)

Product properties are characteristics of composite materials which are not present in the individual phases, but are a result of the interaction between them. An example of a product property is the magneto-electric coupling of two-phase composites. Such composites are also called multiferroic, since they combine two or more ferroic properties. This magneto-electric (ME) coupling can find applications in sensor technology or in magneto-electric data storage devices. Since most ME single-phase materials show such a coupling far below room temperature, the manufacturing of two-phase composites, consisting of a ferroelectric matrix with magnetostrictive inclusions, becomes important. Due to the interaction of both constituents the composites generate a strain-induced ME coupling at room temperature. The ME coupling significantly depends on the microscopic morphology and the ferroic properties of the individual constituents. In order to take both aspects into account, a finite element (FE2) homogenization approach is performed, which combines via a scale bridging the macro- and microscopic level [1]. Thereby, the microscopic morphology is characterized by representative volume elements and the ferroic properties of the phases are described by suitable material models. The typical ferroelectric hysteresis curves are modeled by considering the switching behavior of the spontaneous polarizations of barium titanate unit cells [2], whereas the magnetic hysteresis loops are described by a Preisach operator [3].

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Investigation of localized instabilities of stretching- and bending-dominated truss lattices treated as nonlocal generalized continua

Raphael Nicolas Glaesener (*ETH Zürich, Switzerland*)

14:40

Claire Lestringant (*ETH Zürich, Switzerland*)

Dennis M. Kochmann (*ETH Zürich, Switzerland, California Institute of Technology, Pasadena, USA*)

The advance of new capabilities in additively manufacturing trusses at small scales has created new opportunities in developing random, periodic, or hierarchical truss networks containing millions and more of individual truss members. The behaviour of these metamaterials can be controlled on the microscale by different truss architectures in order to achieve macroscopic pre-defined material properties that cannot be realized with conventional materials. One of the major drawbacks of these truss structures is the immense computational expense required to predict the mechanical response of the large amount of single individual truss members.

Understanding and efficiently modelling localised deformations, instabilities and fracture will increase our ability to predict the mechanical behaviour of architected materials. As the costs for the computational calculation of the mechanical response is increasing rapidly with larger truss structures, advanced and efficient approximation tools are necessary.

We present an extension of the model developed by Kochmann and Desmoulin (1), describing a generalized continuum description of truss lattices based on the (non-)local Cauchy-Born rule, that allows us to bridge between the microscopic representative unit cell and the macroscopic boundary value problem. Separation of scales gives us the capability of accurately representing a large underlying periodic discrete lattice while requiring only a fraction of the degrees of freedom. We extend this model, now considering translational and rotational degrees of freedom to describe linear and nonlinear beam bending, resulting in a higher-order continuum theory on the macroscale. We further present a multi-lattice approach for bending-dominated truss lattices and show that the decomposition of bending-dominated lattices into multiple superimposed Bravais lattices with relative shifts in between leads to an improved performance of the continuum model and a more accurate representation of the mechanics of bending-dominated truss structures. We highlight the accuracy and efficiency of the model by inserting it into finite elements and presenting several benchmark tests also including examples with instabilities and localizations. We also highlight how our continuum description accurately approximates full, discrete truss deformations with only a small fraction of the computational costs.

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Homogenization-based multiscale design of truss metamaterials with controllable effective properties

Bastian Telgen (*ETH Zürich, Switzerland*)

15:00

Dennis M. Kochmann (*ETH Zürich, Switzerland*)

Lattice materials open a large design space with respect to mechanical properties such as stiffness or strength, and weight [1]. Recent and anticipated advances in additive manufacturing techniques are opening the floor for structural integration on a material scale. This poses the need for efficient and robust design approaches. To overcome the excessive computational demand for full-fidelity mechanical characterization of such lattices, homogenization is an effective choice to replace a fully-resolved simulation representing each and every strut and node in the truss by an efficient continuum representation. However, the challenge to bridge between continuum and discrete scale design parameters arises. Projection-based methods [2] have proven to

provide near-optimal results while being computationally efficient, yet restrict the design space and require careful postprocessing on the microscale.

We borrow from crystallography principles and propose a lattice generation procedure that generalizes the design space of general classes of truss networks (including periodic and structurally graded ones) while assuring robust microstructure constructability and printability. The approach is generally applicable to 2D and 3D, bending- and stretching-dominated lattices. In conjunction with a semi-analytical, homogenization-based continuum model that admits effective property prediction without full-scale discrete lattice simulations [3], a generic and efficient exploration of truss lattices is possible. Periodic and graded lattice studies are performed and, embedded in homogenization-based topology optimization, near-optimal lattice-based structures are generated for a variety of load cases.

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Contact between shear-deformable beams with elliptical cross sections to represent dry-woven fabrics

Marco Magliulo (*University of Luxembourg, Luxembourg*)

15:20

Lars Beex (*University of Luxembourg, Luxembourg*)

Andreas Zilian (*University of Luxembourg, Luxembourg*)

Dry-woven fabrics are used in numerous products. To manufacture parts with reinforced plastics for instance, a dry-woven fabric can be placed in a preform and subsequently covered by molten polymer and cured in an autoclave. For the mechanical performances of the final product, it is important how the dry-woven fabric deforms during its placement in the draping tool. In particular, relative displacements of the yarns may occur, which can lead to local variations of the mechanical properties of the final product. These rearrangements in the dry-woven fabrics are largely governed by the contact between the yarns undergoing large displacements and rotations. A mesoscopic model for dry-woven fabrics is formulated in which each yarn is individually represented by a string of beam finite elements together with the contact interactions between yarns. Only one contact scheme for shear-deformable beams with non-circular cross-sections currently exists and it does not allow for beams substantially bending over each other or for parallel beams. A novel contact framework (including Coulomb's friction) for shear-deformable beams with elliptical cross sections has been formulated and will be presented.

Due to its discrete character, the developed framework is computationally expensive if applied in application-scale simulations. A concurrent multiscale method, called the quasi-continuum (QC) method, is therefore employed to reduce the computational cost. This method has mostly been used to alleviate the burden of atomistic lattice computations and has been reformulated to deal with dissipation in structural models and irregular structures. We build on these extensions and show that the multiscale framework is substantially faster than the direct numerical simulations, whilst the introduced numerical error remains acceptably small.

Classification of process induced porosity with topological data analysis

Paul Jäger (*University of Innsbruck, Austria*)

15:40

Roland Traxl (*University of Innsbruck, Austria*)

Roman Lackner (*University of Innsbruck, Austria*)

Effective physical properties of porous materials, such as e.g. permeability, strength, and conductivity, strongly depend on the pore space of the material. Even in case of a similar overall porosity, a physical property may significantly vary as it is vastly depending on the pore-space geometry. With the ongoing developments in x Ray computed tomography (CT), the microstructure has become experimentally accessible, allowing for the investigation of the interconnections between geometric properties of a porous material and its effective properties. For this purpose, two main approaches have been developed in the past:

- First, numerical simulations may be performed employing the 3D image obtained from CT measurements.
- Secondly, the microstructure of the material may be characterized by so-called statistical descriptors which are then used to establish a (semi-) empirical relationship with the desired material property.

For both approaches, two questions remain unanswered:

- (i) Which are the appropriate parameters for capturing the relevant geometrical features of the pore space of the material?
- (ii) What is the minimal size of the domain that fully contains these features?

In this contribution we approach these questions with topological data analysis (TDA), a tool originating from big data analysis being adopted for pore-space characterization in the recent years. TDA essentially captures the 0-D, 1-D, and 2-D homology classes by means of a control parameter, i.e. the distance to the nearest pore-material boundary voxel. The information is then stored in so called persistence bar-codes which are a fingerprint for the material geometry. Following the procedure outlined in [1], TDA is applied to various digital model materials, from single pores (e.g. spheres, tetrahedrons, ...) to connected pore-space geometries (e.g. the overlapping spheres model material).

The influence of the geometry on the persistence bar-codes and the determination of statistical geometrical descriptors such as (i) pore- and grain size distribution, (ii) distribution of pore-throat- and grain-grain-contact radii and (iii) the connectedness of the pore space, from the persistence bar-codes is addressed.

Finally the minimal size of the volume element necessary to capture the full information given by the persistence bar-codes is investigated for the model materials under consideration.

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S08.08 | Multiscales and homogenization

Date: February 21, 2019

17:40-18:40

Room: HS 41

A bottom-up continuum approach of crystal plasticity for the analysis of fcc microwires under torsion

Kolja Zoller (*Karlsruhe Institute of Technology (KIT), Germany*)

17:40

Katrin Schulz (*Karlsruhe Institute of Technology (KIT), Germany*)

Metal forming simulations today are based on classical constitutive descriptions of yield behavior and hardening. Microstructural materials characteristics like grain size or dislocation microstructure are rarely considered and never systematically evolved. In the last years, the striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of plastic deformation processes. However, small-scale approaches which include the microstructure of defects of the material in a discrete way come along with the drawback of very high computational costs. Based on the evolution of dislocation densities in a continuum model, we introduce an efficient numerical strategy for representing the evolution processes as well as the dislocation interactions in a material. Herein, a fully three dimensional set-up is considered, representing the elasto-plastic deformation processes in face centered cubic crystals. Microwires under torsion are studied in order to discuss the underlying physical mechanisms and interactions with respect to discrete dislocation dynamics and gradient plasticity.

Material behavior across scales - grain scale to continuum

Payam Poorsolhjouy (*TU Graz, Austria*)

18:00

Thomas Hochrainer (*TU Graz, Austria*)

Macroscopic behavior of materials is a direct function of their microstructure, and its corresponding micromechanical properties. This is most clear in studying granular (particulate) materials, in which, material's microstructure evolves significantly during the course of loading and will fundamentally alter their load bearing and failure mechanisms. Moreover, granular materials have certain characteristic features which make them harder to study using traditional continuum mechanics models.

To derive the behavior of these materials in a manner that (i) incorporates their microstructure into the macroscopic behavior and (ii) is computationally efficient and therefore applicable to real size engineering problems, we develop an interconnected set of models working at different length scales. We develop Particle Mechanics Approach (PMA), incorporating the nonlocal effects of different contacts at each particle at grain scale. In this manner, we are able to consider the interplay of displacements at different locations on each particle and better predict the behavior of the granular assembly as a whole, particularly at large strains (small porosities). On larger scale and in order to derive a continuum model that can capture the effects of the material's microstructural properties, we develop Granular Micromechanics Approach (GMA) which derives materials' macroscopic behavior through a statistical analysis of the behavior of inter-particle contacts in all generic directions. Through GMA, we are able to, with minimal additional computational demand, capture the effects of load-path dependent anisotropic evolution of microstructure on material's macroscopic behavior¹.

The eventual goal of this research effort is to derive an interconnected hand-shake of models at different length scales cross-feeding each other². This will enable the analysts and designers

to derive results with desired level of fidelity and accuracy. In this manner, the calculated macroscopic behavior of the material will be consistent with true properties of the material at micro-scale.

References:

- 1- Poorsolhjoui, P. and Misra, A., 2017. International Journal of Solids and Structures, 108, pp.139-152.
- 2- Poorsolhjoui, P. and Gonzalez, M., 2018. Mechanics Research Communications, 92, pp. 21-27

Demand-based coupling of the scales in the finite temperature CADD method

Patrick Wurm (*Graz University of Technology, Austria*)

18:20

Manfred Ulz (*Graz University of Technology, Austria*)

Atomistic models (i.e. molecular statics or dynamics) allow one to simulate many material phenomena at high accuracy, but are generally bound to overwhelmingly high computational cost, even for very small systems. However, in many cases, the processes which require atomistic resolution are localized in small subregions of the system, and the remaining regions may be accurately described as a continuum. This motivates the use of multiscale atomistic-to-continuum models.

The coupled atomistic and discrete dislocation (CADD) method is a highly accurate representative of these models. It is designed to study dislocation dynamics and permits the transfer of dislocations across the interface between the atomistic and continuum region. In particular, CADD couples an atomistic analysis with the discrete dislocation formulation of van der Giessen & Needleman.

The continuum model is treated as static or dynamic in the existing finite temperature literature. In these studies, the continuum solution is computed at each microscale timestep (permanent coupling) or at some predefined frequency. In times when there is no deformation happening at the coupling interface or in the continuum, these computations are in vain, as they only convey (possibly unwanted) thermal fluctuations into the continuum.

We therefore propose a new demand-based way of incorporating the continuum scale. By using a very simple and cost-efficient algorithm, we are able to detect deformation near the interface and compute the continuum solution only during these periods. We show in numerical examples that this approach yields results that are of the same quality as in the case of a permanent coupling, but comes with reduced computational cost.

S08.09 | Multiscales and homogenization

Date: February 21, 2019

17:40-18:40

Room: SR 03

A plaque growth model with fast oscillating forcing

Florian Sonner (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

17:40

We consider a simplified model for plaque growth in atherosclerosis, a widespread disease of arteries. The speed of growth is linked to the mechanical stresses exerted by the blood on the wall, creating a two-way coupling between the pulsating blood flow and the growth due to the change in wall geometry. The direct numerical simulation of such a coupled system is infeasible, since significant growth occurs on a time scale of months and years, in contrast to the heart beat on a scale of seconds. In this talk we use temporal multiscale methods to derive an averaging limit system, prove quantitative error bounds to the full model and investigate the limit system and its numerical challenges.

Reduction of round-off errors in chemical reaction systems with different timescales

Axel Ariaan Lukassen (*TU Darmstadt, Germany*)

18:00

A spatially homogeneous gas reaction system is modelled by an ordinary differential equation $z' = f(z)$, $z(0) = z_0$.

Thereby the timescales of the chemical processes usually cover a range from 10^{-9} to 10^2 seconds. Hence, the considered ordinary differential equation is a very stiff system of differential equations. Due to stiffness, there are very large round-off errors in the numerical evaluation of the chemical source term. The evaluation of the chemical source term $f(z)$ requires subtraction and addition of very large numbers due to the fast processes, which results in round-off errors by cancellation. The effect of these round-off errors on the Newton's correction is damped in the directions of the fast processes, but it is retained in the directions of the slow processes or the conserved quantities. Hence, the round-off errors may result in failure of Newton's method. If Newton's method fails, numerical integration methods may require very small step sizes. In order to avoid failure of Newton's method, the occurring round-off errors are reduced. This is achieved by reducing the range of the occurring timescales. In contrast to the quasi-steady state assumption (QSSA) and the partial equilibrium assumption (PEA), the reaction velocity of the fast processes is not set to infinity but is decreased in the presented approach. Thereby the modified reaction velocity guarantees partial equilibrium within the tolerance in the shortest considered time interval of interest.

Mechanical properties assessments of as-cast light alloys predicted by a new size-sensitive variant of Differential Effective Medium theory

Ludmila Radeva Parashkevova (*Bulgarian Academy of Sciences, Bulgaria*)

18:20

Ludmil Drenchev (*Bulgarian Academy of Sciences, Bulgaria*)

The presented analytical approach is aimed to evaluate the mechanical properties of multiphase alloys regarded as "in situ" multiphase composites. The materials of interest are composites with high volume fraction of phases embedded into the matrix. According to the two-steps homogenization procedure adopted, the multiphase Representative Volume Element (RVE) consisting of a matrix and n_f phases is equivalent to a RVE containing n pseudo grains, $n \geq n_f$. Each pseudo-grain is a two-phase composite with predominant non-matrix phase. The new size-sensitive variant of Differential Effective Medium (DEM) homogenization scheme for a two-phase composite is described in closed form solutions for semispherical inclusions. Herein the variant of size-sensitive Mori-Tanaka method is postulated as an explicit homogenization scheme for the dilute inclusion problem, which has been further developed following the ideas of DEM. In this way a special dimensionless term arises being the only trace of Cosserat properties of the initial matrix. This term is regarded as an internal model parameter expressing in average manner the sensitivity of the parent matrix to the presence of inclusions of particular shape and size.

The particular case when the inclusions and the matrix have one and the same bulk modulus is applied to model the elastic behavior of cast Mg alloys with discontinuous precipitations. The analytical solutions obtained for a composite with zero bulk modulus of inclusions are appropriate for modelling of closed cell foams of different kind. The properties predictions of the new modification of DEM are compared with results obtained by the classical DEM method, by other theories and with some experimental data available.

S08.10 | Multiscales and homogenization

Date: February 22, 2019

08:30-10:30

Room: HS 41

Boundary conditions in continuum dislocation dynamics

Thomas Hochrainer (*Technische Universität Graz, Austria*)

08:30

Continuum dislocation dynamics (CDD) is a single crystal strain gradient plasticity theory based exclusively on the evolution of the dislocation density variables. In the current contribution we regard the boundary conditions for these CDD density variables and their fluxes from two perspectives. On the one hand, a Coleman-Noll procedure is employed to obtain thermodynamically consistent bulk evolution equations and boundary conditions for the dislocation density variables of CDD. On the other hand we review classical boundary conditions for the dislocation density tensor as already developed by Kröner and discuss their geometric meaning and implications for the CDD variables and their evolution. This does especially lead to uncommon outflow boundaries at corners which have no counterpart in point particle based flux boundary conditions. Numerical examples highlight the effect of the boundary conditions on the density evolution and deformation behavior in small scale plasticity.

Coupled atomistic-continuum simulation of the mechanical properties of single-layered graphene sheets

Qige Zheng (*University of Kassel, Germany*)

09:10

Jens Wackerfuß (*University of Kassel, Germany*)

Due to the exceptional features of graphene sheets, many research projects are focused on them since they were discovered in 2004 [1]. Besides experiments, also numerical simulations are necessary for studying their mechanical properties. The models which are used in the simulations can be classified into two categories: molecular mechanical models and continuum mechanical models.

Effects on the atomic scale can be described explicitly with molecular mechanical models. However, this type of models is restricted to simulate structures of small sizes. By contrast, large and technical relevant structure can be calculated efficiently with continuum mechanical models. However, these models are not able to describe effects on the atomic scale. A concurrent coupling of an atomistic and a continuum model is a promising strategy to combine the advantages of both methods.

In this work, the modeling of a single-layered graphene sheet is divided into three parts. One is atomistic domain which is simulated with the atomic-scale finite element method (AFEM) [2]. Another is a continuum domain. In this domain, the mechanical properties are investigated by using a finite element based on a nonlocal continuum shell model with a high order strain gradient. To be exact, it is a 4-node 24-degree of freedom (DOF) Mindlin-Reissner shell element with a second order strain gradient [3, 4]. In the third part, a new transitional finite element is developed for smoothing the transition between the atomistic domain and continuum domain. The in-house software dockSIM was used to perform these calculations.

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Investigation of the mechanical behavior of polystyrene using molecular dynamics

Maximilian Ries (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*) 09:30
Paul Steinmann (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)
Sebastian Pfaller (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

Polymers are becoming increasingly important as a design material for solving engineering problems. Usually, their properties are adapted specifically to the demands of the desired application by adding filler particles. Meanwhile, it is possible to manufacture such additives at the size of a few nanometers, which makes an experimental investigation of the mechanisms at the molecular level impossible. Instead, numerical multiscale modeling approaches are used to examine and understand the effects of the nanoparticles. These methods, however, require a precise constitutive model of the constituents of the nanocomposite in order to obtain reasonable and reliable results. The Capriccio method introduced in [1] couples a particle domain with a continuum and is used i.a. to investigate the effects of nano-sized silica additives embedded in atactic polystyrene (PS) [2]. The particles are modeled with molecular dynamics (MD) and so far, a simple hyperelastic constitutive law is used for the continuum description. To further enhance the quality of the results, the material model should be derived directly from pure MD simulations under thermodynamic conditions identical to those used by the Capriccio method. This contribution is a first step in this process and characterizes the material response of pure PS under uniaxial deformation using strain-controlled MD simulations. Therefore, noncyclic and cyclic uniaxial tension and compression tests as well as relaxation and creep simulations are performed on a statistically sufficient number of MD systems. A clear dependency on the magnitude and rate of the applied deformation is identified and, in addition, cyclic softening occurs resulting in equilibrium stress-strain-hystereses. As a result, the present PS exhibits viscoelastic characteristics for small deformations, whereas elastic viscoplasticity is observed for larger strains. The gained insights will provide the basis for the selection of a suitable material model whose parameters will be found in a subsequent parameter optimization.

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[2] Pfaller, S.; Possart, G.; Steinmann, P.; Rahimi, M.; Müller-Plathe, F. & Böhm, M., Investigation of interphase effects in silica-polystyrene nanocomposites based on a hybrid molecular-dynamics–finite-element simulation framework. *Physical Review E*, APS, 2016, 93, 052505.

Modelling atomic scale rearrangements in silica glass under simple shear deformation

Firaz Ebrahim (*RWTH Aachen University, Germany*) 09:50
Franz Bamer (*RWTH Aachen University, Germany*)
Bernd Markert (*RWTH Aachen University, Germany*)

The elementary plastic events in glassy materials are atomic scale rearrangements called shear transformation zones that interact and form shear bands at coarser scales [1]. It is known that the medium-range order of the glass network plays a significant role in the deformation behaviour of glasses [2,3]. Thus, in this study, we investigate the effect of the distribution of the local atomic arrangement on the shear transformations. For this purpose, we use molecular dynamics simulations to subject silica glass to simple shear deformation.

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FFT-based homogenisation accelerated by low-rank approximations

Jaroslav Vondřejc (*Technische Universität Braunschweig, Germany*) 10:10
Dishi Liu (*Technische Universität Braunschweig, Germany*)
Martin Ladecký (*Czech Technical University in Prague, Czech Republic*)
Hermann G. Matthies (*Technische Universität Braunschweig, Germany*)

Fast Fourier transform (FFT) based methods had turned out to be an efficient computational approach for numerical homogenisation. Here this kind of methods are further sped up by incorporating low-rank tensor approximation techniques.

The model problem in homogenisation consists of a scalar linear elliptic variational problem defined in two and three dimensional setting with continuous or discontinuous material coefficients. The problem is solved by using a Fourier Galerkin approach [1] where the solution is approximated by trigonometric polynomials. To overcome the large computational complexity the material coefficients and solution tensor are represented in low rank factorized formats including canonical, Tucker, and tensor train formats. It is shown in this work that these low rank approximations of tensors lead to a significant reduction in computational and memory costs for homogenisation of material with a moderate rank. The advantages of this approach against those using full tensors are demonstrated in some examples.

- [1] J. Vondřejc, “Improved guaranteed computable bounds on homogenized properties of periodic media by the Fourier-Galerkin method with exact integration,” *Int. J. Numer. Methods Eng.*, vol. 107, no. 13, pp. 1106-1135, 2016.

S08.11 | Multiscales and homogenization

Date: February 22, 2019 08:30-10:30
 Room: SR 03

Canonical quasicrystalline metamaterials

Massimiliano Gei (*Cardiff University, United Kingdom*) 08:30
Lorenzo Morini (*Cardiff University, United Kingdom*)
Zhijiang Chen (*Cardiff University, United Kingdom*)

The Floquet-Bloch spectrum of a family of one-dimensional two-phase periodic structured rods generated by a quasicrystalline sequence -such as the Fibonacci recursion rule- is characterised by self-similar stop/pass band layouts and scaling phenomena [1,2,3]. These properties are governed by an invariant function of the circular frequency, the Kohmoto’s invariant, which can be represented as a surface in a suitable three-dimensional space. In general, the traces of the transmission matrices of the family of rods identify orbits on the Kohmoto’s surface [2]. For a set of particular frequencies, the canonical frequencies, the orbits are closed. The condition for the

existence of these frequencies is that a particular ratio between the constitutive parameters of the two phases composing the waveguide is a rational number. We show that for these canonical structures the scaling of the spectrum can be determined analytically performing a linearisation of the orbit concerned. We also show that for frequencies that are not canonical, there are two types of stop bands for the same rod, regular and ultrawide. For both, an analytical estimation is provided.

References

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Local instability driven macroscopic deformations in fibrous networks

Sebastian Domaschke (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zürich, Switzerland*) 08:50

Alexandre Morel (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zürich, Switzerland*)

Giuseppino Fortunato (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland*)

Alexander E. Ehret (*Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland, ETH Zürich, Switzerland*)

Network structures consisting of a multitude of fibres are omnipresent in both biological and technical systems [1]. The fibre segments in between the locations at which fibres interact, e.g., in cross-links, bonds or entanglements, are typically long and slender, so that their mechanical behaviour can be described by structural beam theory. When the network deforms, the loads on the single fibre segments are widely distributed from compressive to tensile states, even if the macroscopic deformations are homogeneous, and even if affinity is assumed. A property of beams under compression is the buckling instability occurring at a certain compression threshold leading to a dynamic change in beam configuration. Local instabilities were identified for several materials, e.g., Lüders banding in low carbon steels [2], buckling in foams [3] and honeycomb structures [4], and were associated with extreme and unexpected macroscopic mechanical responses.

In the present contribution, the effect of the buckling instability on the macroscopic behaviour of fibrous networks is demonstrated. To this end, an affine analytical model was developed first. The approach predicts drastic out-of-plane deformations of the network, which are highly dependent on the segments' aspect ratios, i.e. their length normalised by the diameter. Uniaxial tension tests and scanning electron microscopy on electrospun non-woven materials, which have growing use in biomedical and technical applications [5], confirmed the predicted behaviour. Finally, a multiscale model [6] based on 3D representative volume elements (RVEs) of electrospun networks was used to further rationalise these results in detailed finite element simulations.

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Maximum-entropy approximants for numerical energy relaxation and associated microstructure formation in problems with non-convex energetic potentials

Siddhant Kumar (*California Institute of Technology, USA, ETH Zurich, Switzerland*) 09:10

Vidyasagar Ananthan (*California Institute of Technology, USA, ETH Zurich, Switzerland*)

Dennis M. Kochmann (*California Institute of Technology, USA, ETH Zurich, Switzerland*)

Energy-minimizing microstructures and patterns naturally emerge in problems with non-quasiconvex potential energy landscapes such as those associated with phase transformations, deformation twinning, finite-strain crystal plasticity, etc. Such microstructural patterns can be theoretically linked to the quasiconvex hull of the associated non-(quasi)convex energy potentials. Due to the nonlocal nature of the notion of quasiconvexity, quasiconvexification of the energy density in such problems has traditionally been limited to (semi)analytical techniques such as identifying matching upper and lower bounds by using, e.g., recursive lamination and polyconvexification for the upper and lower bounds, respectively. Numerical techniques such as the finite element method are severely limited by their ill-conditioning, resulting from the loss of convexity; they have also been restricted to geometrically simple problems, often times assuming two-dimensional situations. We present a new numerical avenue based on meshless maximum-entropy (max-ent) approximants, whose results are compared to those of Fourier spectral analysis to tackle quasiconvexification of complex material models in three dimensions. Both max-ent and Fourier spectral methods are compared to the finite element method as a baseline to showcase their ability to solve a wider range of quasiconvexification problems with superior accuracy. Numerical experiments are conducted to predict the quasiconvex envelope of (i) the Saint Venant-Kirchhoff material model under simultaneous compression and shear load, and (ii) multi-well phase transformation models. While the spectral technique can capture microstructural patterns at intriguingly high resolution, max-ent is superior at numerically approximating the quasiconvex hull. To gain insight into the errors of all three numerical techniques, we present a simple analytical study of the general limitations of numerical methods in the context of quasiconvexification for the special case of laminate-type microstructures such as those found in the phase-transformation model.

Innovative characterization and multiscale modeling of dental cement pastes

Petr Dohnalik (*TU Wien - Vienna University of Technology, Austria*) 09:30

Bernhard Pichler (*TU Wien - Vienna University of Technology, Austria*)

Christian Hellmich (*TU Wien - Vienna University of Technology, Austria*)

In dentistry, cement pastes are used for root-end filling, perforation repair, pulp capping, apexification, and sealing [1]. On the market, these materials are referred to as Mineral Trioxide Aggregate, abbreviated as MTA. The main hydraulic constituent of dental cements is typically tricalcium silicate. Radiopacity is ensured by mixing the binder either with bismuth oxide or with zirconium oxide. In addition, a very fine ground limestone filler is frequently added to the powder-type raw material. In order to optimize properties of dental cement pastes, accelerators and superplasticizers are added to the mixing water. Important requirements in dentistry are that the freshly mixed material must be workable for a few minutes and that it hardens rather quickly thereafter, such that close-to-final strength values are reached already one day after production. This is very different to construction cements which are workable for much longer periods of time, which are transforming from a gel-like liquid suspension into a solid material

a few hours after mixing, and which exhibit significant hardening during several weeks. The future goal of the present research is to develop a predictive multiscale model for the early-age evolution of the uniaxial compressive strength of dental cement pastes, by analogy to the model described in [2]. The latter was validated in the field of construction cements. The model allows for studying the sensitivity of the macroscopic compressive strength with respect to changes regarding the volumetric dosages and the mechanical properties of the individual microstructural constituents. This provides the motivation to carry out microstructural characterization of dental cement pastes. As for well-hydrated (= mature) materials, a grid-nanoindentation study is carried out. Volumetric dosages and mechanical properties of the individual microstructural constituents are determined based on deconvolution of histograms of indentation modulus and hardness. The obtained results provide the motivation to characterize the early-age hydration kinetics, in order to gain quantitative insight into the evolution of the materials from the freshly mixed state to mature material stages. In this context, innovative approaches to quasi-isothermal differential calorimetry and to quasi-adiabatic calorimetry are currently developed. The present contribution refers to the lessons learned from the research activities carried out so far.

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A spatiotemporal non-local elastodynamic homogenization for composites

Linjuan Wang (*Peking University, P. R. China*)

09:50

Jifeng Xu (*Beijing Aeronautical Science and Technology Research Institute, P.R. China*)

Jianxiang Wang (*Peking University, P. R. China*)

Bhushan L Karihaloo (*Cardiff University, UK*)

The conventional micromechanical schemes of homogenization give local-form effective properties of composites, and the governing equation for the overall behaviour of composites is thus expressed in a local form that does not involve a characteristic length scale and a time scale. In particular, conventional micromechanical schemes do not give the details of motions of the constituents of composites at the microscale. Based on the moving average concept, we develop a spatiotemporal non-local elastodynamic homogenization formulation for composites composed of conventional local elastic constituents. It is demonstrated that the effective stress, momentum density and body force all exhibit spatiotemporal non-locality due to the differences of the densities and stiffnesses of the constituents of the composite, and it also can reduce to the forms of the previous non-local theories under relevant conditions. Both a characteristic length scale and a time scale naturally emerge from the derivation. The dispersion relations given by the formulation contain an optical branch and an acoustic branch, whereas the previous spatial non-local formulations only give the acoustic branch. The theory has implications in modeling the response of composites involving high gradients of field quantities, and high-frequency dynamic problems. Due to the mathematical analogy of general diffusion problems, the current analysis can be readily applied to other multi-field coupled mechanical problems.

S09 | Laminar flows and transition

Organiser: Bruno Eckhardt (*Philipps-Universität Marburg, Germany*)
Björn Hof (*Institute of Science and Technology Austria (IST Austria), Austria*)

S09.01 | Laminar flows and transition

Date: February 19, 2019
Room: HS 03

08:30-10:30

A network of invariant solutions underlying spatio-temporal patterns in inclined layer convection

Tobias M. Schneider (*EPFL - Swiss Federal Institute of Technology Lausanne, Switzerland*) 08:30

Thermal convection in a fluid between two horizontal plates, a lower hot plate and an upper cold plate, exhibits chaotic dynamics and turbulence. If such a convection cell is inclined against gravity, buoyancy forces drive hot and cold fluid up and down the incline leading to a shear flow in the base state and the emergence of complex dynamics and spatio-temporal patterns.

We study the dynamics of inclined layer convection (ILC) using a fully nonlinear dynamical systems approach based on a state space analysis of the governing equations. Exploiting the computational power of highly parallelized numerical continuation tools based on matrix-free Newton methods, we compute a collection of invariant solutions of ILC and discuss their bifurcation structure. Specifically, fixed points, travelling waves, periodic orbits and heteroclinic orbits will be shown. At intermediate angles of inclination, we demonstrate how a simple network of invariant solutions guides moderately complex dynamics. The complexity of the dynamics increases with the intensity of the basic shear flow. At high inclination angles, localized patches of weakly turbulent convection within a background of straight longitudinal convection rolls are observed. We present exact invariant solutions capturing both the dynamics and the spatial localization of these so-called transverse bursts.

This work is supported by the Swiss National Science Foundation under grant no. 200021-160088

Dimension of the attractor in weakly turbulent Taylor-Couette flow

Raphael Gerlach (*Paderborn University, Germany*) 09:10
Michael Dellnitz (*Paderborn University, Germany*)
Daniel Feldmann (*University of Bremen, Germany*)
Marc Avila (*University of Bremen, Germany*)

For many years observations have been used to reconstruct the dynamics of turbulent flows. In 1987 Brandstätter & Swinney observed velocity time series at selected points of their Taylor-Couette experiment and used time-delay embeddings to reconstruct the underlying attractor, which is justified by several embedding results. For finite dimensional dynamical systems Takens (1981) and Sauer et. al (1991). proved that the so-called delay coordinate map is generically (in the sense of prevalence respectively) one-to-one on the attractor. Furthermore, Hunt & Kaloshin (1999) and Robinson (2005) extended these results for the infinite dimensional setting. This technique allows one to determine the complexity of the flow by computing or estimating the dimension of the embedded attractor.

In our work we perform direct numerical simulations of a minimal flow unit of the Taylor-Couette system for several Reynolds numbers and observe velocity time series and their FFTs as well as integral quantities that account for the drift in the azimuthal/streamwise direction. Thus, we are able to reduce the dimension by one for the laminar regime (at least). For example, in Brandstätter & Swinney the modulated wavy flow (MWF) has a dimension of two, whereas in our analysis it has a dimension of one (seen in a co-moving frame it is a periodic orbit).

To compare our results with Brandstätter & Swinney and improve them we determine the dimension of the embedded attractor using different methods. To this end, we compute the box-counting dimension with the set-oriented methods implemented in GAIO (cf. Dellnitz, Froyland, Junge 2001) as well as the correlation dimension with the software package TISEAN (cf. Hegger, Kantz, Schreiber 1999). In addition to that we find the intrinsic dimension by using a diffusion maps based approach (cf. Berry, Harlim 2016). With this in mind we track the bifurcations - and therefore the route to turbulence - as the Reynolds number increases.

For the laminar flow we observe that the number of peaks in the power spectra match with our computed dimensions for all methods. With the consideration of the drift we find a fixpoint that first bifurcates into a periodic solution (MWF) and then into a 2-torus. In the weakly turbulent regime, however, the box-counting algorithm fails to deliver meaningful results due to the huge amount of needed data in fairly high embedding dimensions. Nonetheless TISEAN and diffusion maps give reliable results and we find a fractal dimension of approximately 4.5 for the weakly turbulent attractor.

Dynamic feedback control of edge states in plane Poiseuille flow

Bruno Eckhardt (*Philipps-Universität Marburg, Germany*)

09:30

Florian Knierim (*Philipps-Universität Marburg, Germany*)

Moritz Linkmann (*Philipps-Universität Marburg, Germany*)

The transition to turbulence in many wall-bounded parallel shear flows, such as pipe or plane Poiseuille flow, is connected to the presence of a lower-dimensional manifold in state space, the edge of chaos, which distinguishes between initial conditions resulting in laminar or turbulent flow. States on the edge manifold have thus at least one unstable direction, and the dynamics will not remain confined to it. However, feedback stabilisation method can be used to remove the effect of the unstable direction, as demonstrated for pipe flow by Willis et al JFM 2017. Here, we focus on similar strategies in plane Poiseuille flow. We investigate the effect of a dynamic pressure-based feedback control on the stable and unstable directions in order to stabilise states on the edge.

Asymptotic suction boundary layer: alternative linear and weakly non-modal stability modes

Alparslan Yalcin (*Technische Universität Darmstadt, Germany*)

09:50

Martin Oberlack (*Technische Universität Darmstadt, Germany*)

According to Kolmogorov's theory, turbulent flows are characterized by a cascade of eddies where kinetic energy is transferred from larger to smaller scales and eventually dissipated into heat. For a variety of turbulent flows, however, it is observed that very large-scale, coherent structures, so called turbulent superstructures, turn out to be rather persistent. These turbulent superstructures play a crucial role in the global mass, heat and momentum transport, but they have yet to be understood entirely.

A prototypical flow for this is the turbulent plane Couette flow, which contains roll-type superstructures in streamwise direction that can be tracked down to the instability modes of the laminar case. Based on this observation, the assumption is made that other types of turbulent

flows feature similar linkages between instability modes and resulting very large-scale structures in the turbulent flow field.

In recent numerical studies it was shown that, although different in structure, very large-scale turbulent streamwise motions may also exist in the Asymptotic Suction Boundary Layer (ASBL) (see e.g. Schlatter and Örlü, 2011, Khapko, Kreilos, Schlatter, Duguet, Eckhardt and Henningsson, 2013 or Bobke, Örlü and Schlatter, 2015).

Based on the fact, that for some flows footprints of the linear unstable modes are observed as turbulent superstructures, linear stability analysis (LSA) was conducted for the ASBL utilizing the classical normal-mode ansatz as well as two new symmetry-induced non-modal ansatz functions. Based on this, an extended set of Orr-Sommerfeld equations was derived for all the cases for which exact solutions in terms of HeunC and hypergeometric functions were generated. The resulting eigenvalue problem provides deep insights on the linear stability characteristics of the ASBL flow.

For the laminar case, however, non-modal algebraic growth is witnessed for large enough disturbance amplitudes, due to which so-called bypass transition occurs at Reynolds numbers of around $Re=300$, which is about two orders lower than the critical Reynolds number postulated by the linear stability analysis. These observations motivate stability analysis with non-modal ansatz functions.

Lie symmetry analysis of the inviscid formulation of the linearized Navier-Stokes equation revealed an additional symmetry on top of classical translation and scaling symmetries, based on which two new non-modal ansatz functions were derived for the ASBL. It is believed that via the application of these ansatz functions new insights can be gained on the laminar-turbulent transition. The ensuing results will be compared to the ones obtained by the LSA conducted with the normal-mode ansatz.

Symmetry-induced unstable modes and transient growth in a Taylor-Couette type model problem

Tim Gebler (*Technische Universität Darmstadt, Germany*)

10:10

Martin Oberlack (*Technische Universität Darmstadt, Germany*)

The Taylor-Couette flow is a paradigmatic system to study the stability of rotating shear flows. In linear stability theory, the assumption of wavelike disturbances (normal-mode ansatz) reduces the stability analysis to solving an eigenvalue problem of ODE type. However, even if all eigenvalues signify stability, transition to turbulence can occur. A possible explanation is the non-normality of the eigenfunctions, which for early times in the transition process, leads to a transient growth and appears to admit an algebraic growth rate.

Independent of this, it has been shown by the present group that the normal-mode ansatz has its basis in symmetries and, moreover, that many classical shear flows admit new symmetry induced eigenfunctions with algebraic growth in time. Using a newly found symmetry-based non-modal ansatz, it is possible to formulate an eigenvalue problem for a two-dimensional Taylor-Couette type flow, where this flow "lives" in a very special domain, where the outer radius tends towards infinity and the inner cylinder is a thin wire. By introducing an additional coordinate transform, we find an analytical solution of the eigenfunctions for a continuous spectrum of eigenvalues. Finally, new unstable 2D modes with algebraic growth in time are identified.

Here, we present a comparison of our non-modal ansatz with the normal mode stability analysis on the special domain defined above. Therefore, the same coordinate transform was applied to the normal mode problem, giving rise to the corresponding eigenvalue problem on the same two-dimensional domain. An analytical expression for the stability is derived thereof. The identified modes are compared with those of the symmetry-induced ansatz.

Although instabilities in a Taylor-Couette system result in 3D vortex structures, we believe that 2D modes give new insights in fundamental instability mechanisms in rotational shear flow.

Although the flow lives on a special infinite domain, that does not correspond to the classical Taylor-Couette geometry, we believe that our new ansatz contributes to the understanding of the stability of the two-dimensional Taylor-Couette type flow. The reason is, that we will also present a new approach to calculate the optimal growth of perturbations in Taylor-Couette flow. This new technique has its roots in Fokas method. Compared with existing approaches, we are able to derive an integral form of the eigenfunctions and to formulate an equivalent optimization problem. Further, the Fokas method may allow us to map the infinite domain to the classical Taylor-Couette geometry.

S09.02 | Laminar flows and transition

Date: February 19, 2019

16:30-18:30

Room: HS 03

Probing transition to turbulence and low-drag turbulent states in channel flow using wall shear stress signals

Rishav Agrawal (*University of Liverpool, United Kingdom*)

16:30

Henry Ng (*University of Liverpool, United Kingdom*)

David Dennis (*University of Liverpool, United Kingdom*)

Robert John Poole (*University of Liverpool, United Kingdom*)

We use a combination of flow visualisation, velocity measurement via laser Doppler velocimetry and wall shear stress signals using a series of “hot-film” probes to investigate experimentally both the transition to turbulence in a channel-flow facility and low-drag turbulent states over a range of Reynolds numbers. We find the hot-film wall shear stress probes are particularly useful and enable us to identify the onset of transition and, via cross-correlations between different probes, detailed information on the dynamics of the transitional events. At higher Reynolds numbers, where the flow is turbulent and large-scale intermittency absent, we use the wall shear stress data to investigate “low drag” events using conditional averaging of the velocity field. In so doing, we are able to reveal potential connections with both exact coherent states from the literature and, in terms of the mean velocity profile, similarities with “drag-reduced” flow usually only observed when polymeric or surfactant additives are added to the flow.

Power-law scaling of friction in pipe flow

Davide Scarselli (*IST Austria, Austria*)

17:10

José Lopez (*IST Austria, Austria*)

Balachandra Suri (*IST Austria, Austria*)

Björn Hof (*IST Austria, Austria*)

Wall-bounded turbulent flows are commonly encountered in many applications where accurate predictions of the skin friction are needed. Despite the simplicity of the problem, there is still some disagreement on how friction scales with the Reynolds number and how turbulence affects it, even in simple flow geometries such as the flow through a pipe.

The idea of a power-law friction was firstly advanced by Blasius [1] as an empirical fit to available experimental data for pipes, for a Reynolds number (based on mean velocity and pipe diameter) up to 10^5 . Subsequently, new experiments [2] at higher Reynolds showed that friction was progressively deviating from a power-law behavior and the focus shifted on finding a universal friction law. Von Karman [3] proposed one such formula that was able to fit data for all the Reynolds available, based on the famous logarithmic law of the mean velocity. In the following years, a great deal of effort has been spent to improve the von Karman law although little

attention was devoted to investigating friction for Reynolds numbers where the empirical power law was still accurate.

With a series of carefully designed experiments and highly resolved direct numerical simulations, we accurately explore the behavior of friction in pipes for Reynolds 5000 to 140 000. Our results show that for $Re < 80\,000$ friction is indeed better approximated by a power law, instead of the von Kármán formula. In addition, in line with a previous study [4], we demonstrate theoretically that a power law scaling arises from a simple balance between production and dissipation. Finally, we investigate the physical mechanisms responsible for the deviation from a simple power law and we show how large scale motions affect friction as the Reynolds number increases.

[1] Blasius, H. (1913). Das Ähnlichkeitsgesetz bei Reibungsvorgängen in Flüssigkeiten. In Mitteilungen über Forschungsarbeiten auf dem Gebiete des Ingenieurwesens (pp. 1-41). Springer, Berlin, Heidelberg.

[2] Nikuradse, J. (1930). Über turbulente Wasserströmungen in geraden Röhren bei sehr grossen Reynoldsschen Zahlen. In Vorträge aus dem Gebiete der Aerodynamik und verwandter Gebiete (pp. 63-69). Springer, Berlin, Heidelberg.

[3] Von Kármán, T. (1930). Nachrichten von der Gesellschaft der Wissenschaften zu Göttingen. Mathematisch-Physikalische Klasse, Fachgruppe I (Mathematik), 5, 58.

[4] Gioia, G., & Chakraborty, P. (2006). Turbulent friction in rough pipes and the energy spectrum of the phenomenological theory. Physical review letters, 96(4), 044502.

Universality of the transition to turbulence in Couette flow

Lukasz Klotz (*Institute of Science and Technology, Austria*)

17:30

Grégoire Lemoult (*Institute of Science and Technology, Austria*)

Björn Hof (*Institute of Science and Technology, Austria*)

Turbulence is one of the most frequently encountered non-equilibrium phenomena in nature. Here we study the transition to turbulence in linearly stable Couette flow. Recently, Lemoult et al. (2016) reported that in this flow turbulence first becomes sustained at a second order phase transition, which falls into the directed percolation universality class. Thus, the interplay between the laminar and turbulent phases can be characterized by universal critical exponents. This also indicates that the complex laminar-turbulent patterns observed in Couette flow result from short-range interactions. We present the results obtained in a new experimental set-up with larger aspect ratio, which enables us to study the dynamics of the turbulent phase in more detail. In particular we determine five power law exponents close to the critical point which are measured independently. All five exponents are in very good agreement with the directed percolation universality class.

References:

G. Lemoult, L. Shi, K. Avila, S. V. Jalikop, M. Avila, B. Hof, 2017, "Directed percolation phase transition to sustained turbulence in Couette flow", Nature Physics, 2016, vol. 12, 254-258

Percolation as a high-precision measurement tool for the laminar-turbulent boundary layer transition on an airfoil

Björn Espenhahn (*University of Oldenburg, Germany*)

17:50

Dominik Traphan (*University of Oldenburg, Germany*)

Tom T.B. Wester (*University of Oldenburg, Germany*)

Gerd Gülker (*University of Oldenburg, Germany*)

Joachim Peinke (*University of Oldenburg, Germany*)

The transition from laminar to turbulent is a highly unsteady phenomenon. It drastically changes the behavior of the flow and therefore the energy transport. Nevertheless, the laminar-turbulent

transition is not yet fully understood and cannot be described completely by now. Based on Pomeau’s conjecture (1986) the laminar-turbulent transition belongs to one universality class of directed percolation.

Recently, Traphan et al.(2018) found out, that the onset of a laminar separation bubble (LSB) on an airfoil is consistent with the directed percolation theory. They introduced a possible characterization of the turbulent behaviour by a certain set of critical exponents belonging to the universality class of the (1+1) D directed percolation. Additionally, using percolation as a measurement tool, the onset of the LSB is determined with an uncertainty of less than 1% of the chord length. Such a high precision was rarely obtained in a turbulent system before.

In the present study, these investigations are extended to the laminar-turbulent transition instead of the LSB. For verifying the laminar-turbulent transition reflecting directed percolation, the boundary layer of an airfoil is examined by high-speed stereoscopic PIV, ensuring high spatial and temporal resolutions. This leads to a sufficient resolution for detecting the onset of the laminar-turbulent transition. At the transition point, turbulent cells emerge. Their distribution in terms of spatio-temporal size is then compared with the set of critical exponents, given by directed percolation. First investigations on the laminar-turbulent transition confirm the characteristics of the (1+1)D directed percolation and show similar results compared with the LSB. Further, the onset of the laminar-turbulent transition can be specified with the same high precision of better than 1%. These results indicate, that Pomeau’s conjecture is true for the LSB, as well as for the laminar-turbulent transition, both in technical flows about airfoils.

Three-dimensional flow in a shear-driven cube

Pierre-Emmanuel des Bosc (*TU Wien, Austria*)

18:10

Hendrik C. Kuhlmann (*TU Wien, Austria*)

The incompressible flow in a cubic container (edge length L) is investigated, which is driven by a constant shear stress τ parallel to the edge and acting on one face of the cube. The problem is related to the classical benchmark of the flow in a lid-driven cube. The spectral element solver NEK5000 is used to fully resolve the laminar flow, using $12 \times 12 \times 12$ elements of polynomial degree $P = 6$ for the velocity and $P = 4$ for the pressure. At small Reynolds numbers $Re = (L^2/\nu^2)\tau$ the flow is steady and symmetric with respect to the symmetry plane of the problem. At $Re_{c1} = 53400 + / - 100$ the mirror symmetry is broken and the bifurcating flow becomes unsymmetric and steady. The steady bifurcation is studied using the BoostConv algorithm which also allows to recover the unstable symmetric solution. By restricting the solutions to the subspace of symmetric solutions be shown that the symmetric basic state remains stable in the symmetric subspace, but gets unstable in the full phase space. At the even higher Reynolds number $Re_{c2} = 55750 + / - 250$ a Hopf bifurcation arises. The properties of the three distinct flow states are discussed and compared to the sequence of bifurcations recently found for the lid-driven cavity. The results show that the scenario of transition to turbulence is quite different in both systems.

S09.03 | Laminar flows and transition

Date: February 20, 2019

14:00-16:00

Room: HS 03

Transport of electrically charged particles in transonic and supersonic gas flows

Laurent Bernier (*Technische Universität Berlin, Germany*)

14:00

Philipp Krahe (*Technische Universität Berlin, Germany*)

Julius Reiss (*Technische Universität Berlin, Germany*)

Mass spectrometry usually relies on high vacuum chambers containing free ions. One technique to produce such particles is the electrospray ionization (ESI), which operate at atmospheric pressure. This strong pressure difference and the resulting gas flow is used to transport the ions from the source into the lower pressure areas of the machine.

The aim of the presented project is to offer a detailed insight into the transfer of the ions in the first two stages, the inlet capillary and the first pumping chamber. The trajectory of the ions, including the influence of the gas flow, the external electric fields, and the Coulomb's interaction, is simulated alongside a detailed gas flow simulation. The latter is complex in itself, as the strong acceleration due to the pressure gradient is related to sonic conditions in the capillary and results in an underexpanded jet in the first chamber, where complex geometries can be found.

For the inlet capillary, a detailed analysis of the gas flow is performed. This includes the influence of geometrical parameters such as length and diameter, as well as the operating conditions, represented by the temperature of the capillary walls. The different resulting flows and their consequences on the transport of the ions are presented. The impact of the considered ions species is also taken into account, as this has an impact on transmission efficiency.

The first pumping chamber is further presented, with the example of a complex ion guiding system, for which results of preliminary simulations are shown.

The numerical framework results from a clear separation between the code dedicated to the gas flow calculation and the one dealing with the ion transport. This allows a certain flexibility in the combination, the ion code having the ability to be connected with different gas flow solvers. The communication between both sides occurs via the parallelization framework, using the Message Passing Interface.

Transformation of tribological modelling of squeeze flows to simulate the flow of highly viscous adhesives and sealants in manufacturing processes

Michael Müller (*Braunschweig University of Technology, Germany*)

14:20

Yan Tong (*Braunschweig University of Technology, Germany*)

Till Vallée (*Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Germany*)

Holger Fricke (*Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Germany*)

In bonding processes, the main influence for the resulting adhesive distribution after pressing is the adhesive used on the surfaces to be bonded, the adhesive's initial distribution pattern and the pressing process itself. Therein, a particular issue is the creation, and transport, of air bubbles during manufacturing that strongly influences the joint's strength. Numerical simulation of the flow in these processes is most commonly based on Computational Fluid Dynamics (CFD). In the general 3D case, these simulations are very complex, time-consuming and are therefore rarely performed. Particular challenges stem from the usually thin layer of adhesive, which in

turn requires extremely fine meshes, thus increasing the already high modelling cost. From another scientific discipline, the theory of lubricated friction contacts, it is known that the flow in narrow gaps can be approximated with the Reynolds equation, which does not discretize the height direction, thus significantly reducing overall modelling costs. For frictional contacts, the aforementioned simplification is numerically very efficient with respect to computational effort and convergence, and results in solutions very close to 3D-CFD simulations. As an extension of the Reynolds equation, in recent years the research group at the TU Braunschweig has developed a model that takes into account not only the efficient calculation of the interaction between flow and pressure build-up but also the dynamics in gaps that are only partially filled with fluids. This so-called PFG (Partially Filled Gaps) model is also able to explicitly describe the movement of air inclusions.

This paper discusses the potential of this approach as a tool for describing the adhesive flows during pressing. It demonstrates that the theory of lubricated friction contacts is an interesting concept for a wide range of pressing process simulations.

Simulation of the flow behavior of wood-polymer composites in extrusion dies

Fabian Liese (*University of Kassel, Germany*)

14:40

Olaf Wunsch (*University of Kassel, Germany*)

By adding different fillers to polymers, both the mechanical and optical properties of the composite can be influenced. The addition of wood flour or fibers results in wood-polymer composites (WPC), which are industrially processed into deckings by means of an extrusion process. As part of this project, the melt of HDPE and fine wood flour is extruded into a square hollow profile. By means of thermo-rheological measurements, the shear thinning behavior, yield points as well as the solidification behavior of WPC at various degrees of filling levels of the wood and different temperatures could be determined. From fill levels above 60 % wood, removal by means of a crawler belt is no longer possible due to the low elongation, so that a partial solidification of the melt prior to exiting the extrusion die by cooling is necessary. In addition to solidification, wall slip effects in the area of cooling occur as a function of shear stress, which could also be measured and modeled using the Mooney method [1]. This contribution deals with the numerical flow field calculations of such WPC in special extrusion dies. From the thermo-rheological data a viscoelastic material model is created. The aims of the numerical simulations with OpenFOAM are to reduce pressure loss and create a uniform temperature field at the outlet. Different parameters such as the mass flow of the melt and the temperature of the cooling medium are varied.

[1] Mooney, M., Explicit Formulas for Slip and Fluidity, *J.Rheol.*, 2, 210.1931

Purely viscoelastic linear instability in plane Couette flow

Gunnar Martin Lellep (*Philipps University Marburg, Germany*)

15:00

Bruno Eckhardt (*Philipps University Marburg, Germany*)

Alexander Morozov (*University of Edinburgh, Scotland*)

Purely elastic turbulence (PET) refers to chaotic dynamics in overdamped polymer solutions in the absence of inertia. Its origins and the mechanisms underlying its dynamics are largely unknown. In order to explore a possible relation to instabilities, we here study the linear stability of the Oldroyd-B model in a plane Couette flow geometry with free-slip boundary conditions (BCs). The free-slip BCs reduce the influence of the walls and shift the focus on the effects of elasticity. Increasing the Weissenberg number, we find a linear instability to a 2D flow state. The eigenvalue spectrum bears a striking resemblance to the spectrum of plane Couette flow of Oldroyd-B fluids with no-slip BCs, which consists of two continuous lines of eigenvalues and a pair of complex conjugate eigenvalues. In the case of rigid BCs, the two isolated eigenvalues

(known as Gorodtsov-Leonov modes) are linearly stable whereas here they become unstable. The connection between the isolated modes for the two cases is demonstrated by a homotopy in the BCs. The behaviour of the viscoelastic system differs from its Newtonian counterpart, as the latter does not exhibit a change in stability upon a change in the BCs. The instability described here is driven by elasticity and disappears with increasing inertia. It should provide a good starting point for further theoretical studies of PET.

A phase transition to condensate formation in two-dimensional turbulence

Moritz Linkmann (*Philipps-University of Marburg, Germany*)

15:20

Manuel Hohmann (*Philipps-University of Marburg, Germany*)

Guido Boffetta (*University of Turin, Italy*)

M. Cristina Marchetti (*University of California Santa Barbara, USA*)

Bruno Eckhardt (*Philipps-University of Marburg, Germany*)

Two-dimensional (2d) and quasi-2d flows occur at macro- and mesoscale in a variety of physical systems. Examples include stratified layers in Earth's atmosphere and the ocean, soap films and more recently also dense bacterial suspensions, where the collective motion of microswimmers induces patterns of mesoscale vortices. A characteristic feature of 2d turbulence is the occurrence of an inverse energy cascade. In absence of large-scale friction the inverse energy cascade results in the formation of large-scale coherent structures, so-called condensates. We here study the formation of the condensate as a function of the kind and amplitude of the forcing. Direct numerical simulations show that the condensate does not appear gradually but in a phase transition. For prescribed energy dissipation the transition is second order; for active matter, where the forcing is due to a small-scale instability, the transition is first order. The phase transition separates two markedly different types of 2d turbulence: in turbulence with a condensate, energy input is predominantly balanced by dissipation in the condensate and intermediate scales follow an inertial cascade; without a condensate dissipation is spread over the intermediate scales and the properties of the energy transfer are noticeably different and non-universal.

S10 | Turbulence and reactive flows

Organiser: Bettina Frohnappel (*Karlsruhe Institute of Technology (KIT), Germany*)
Arne Scholtissek (*Technische Universität Darmstadt, Germany*)

S10.01 | Turbulence and reactive flows

Date: February 20, 2019
Room: HS 03

16:30-18:30

Pulverised fuel flames: fully-resolved and Euler-Lagrange simulations

Oliver Thomas Stein (*University of Stuttgart, Germany*)

16:30

Pulverised solid fuel combustion plays a critical role for global energy conversion. However, the pollutant emission and climate change impact of solid fuel flames, particularly coal, may be significant and substantial research efforts towards an increased understanding of the underlying physical and chemical phenomena are required to improve the fuel conversion process. Despite recent experimental advances in combustion diagnostics it remains difficult to obtain reliable, non-intrusive measurement data, which is due to the hostile environment that prevails in solid fuel flames. Numerical simulation provides a suitable alternative tool for investigating fundamental aspects of solid fuel conversion. Here we focus on detailed numerical simulations of the principal physico-chemical processes occurring in pulverised fuel combustion, namely fluid transport, particle heating, devolatilization, ignition, volatile combustion and char conversion. Results from two simulation approaches are discussed, a) fully-resolved simulations, where all relevant scales of the flow -including the particle boundary layers- and the flame are resolved and, b) Euler-Lagrange simulations, where the fluid phase is fully resolved, but the dispersed solid phase is treated as a set of Lagrangian point-particles.

The fully-resolved simulations serve to obtain a fundamental understanding of the ignition and burning of single particles and small particle groups. The governing parameters that influence these processes are examined, namely the inter-particle spacing L_x and the particle Reynolds number Re_ρ , as well as the presence of a locally laminar or turbulent flow environment. These parameters may strongly affect the resulting flame structure and burning mode, ranging from single particle burning to group combustion. The fully-resolved simulations provide mixture fraction distributions in the particle wake, and indicate limitations of standard flamelet models and film theory to predict highly strained volatile flames. First results from an improved modelling approach that makes use of a detailed, yet general kinetic approach for solid fuel conversion are also discussed.

Since fully-resolved simulations are limited to small numbers of particles, the Euler-Lagrange approach with a resolved carrier phase provides a suitable alternative for the detailed study of larger solid fuel flames. To this end, we present recent results from the carrier-phase DNS of coal particle ignition and burning in a three-dimensional turbulent mixing layer. The simulation data is analysed in terms of ignition criteria and flame index, where ignition occurs for locally lean conditions, and both premixed and non-premixed flame regions can be identified. Furthermore, the results are assessed in the context of flamelet/progress variable (FPV) modelling.

Adjoint-based sensitivity analysis of complex combustion models

Mathias Lemke (*Technische Universität Berlin, Germany*)

17:10

Liming Cai (*RWTH Aachen University, Germany*)

Julius Reiss (*Technische Universität Berlin, Germany*)

Heinz Pitsch (*RWTH Aachen University, Germany*)

Jörn Sesterhenn (*Technische Universität Berlin, Germany*)

An adjoint-based approach for the sensitivity analysis of complex reaction mechanisms is presented. It builds purely on the evaluation of the governing primal equations. No adjoint equations have to be derived explicitly. Instead, the required adjoint operator is constructed numerically on the fly in contrast to algorithmic/automated differentiation. The approach can be utilized for various kinetic models and in existing codes with minimal implementation effort. All dependencies on the state and on model parameters are fully evaluated without simplifications. Thus, also non-standard rate laws can be considered with minimal effort. In comparison to the standard brute-force finite-difference technique, the advantages of the approach are two-fold: first, the approach derives exact gradients for the parameters and is exempt from the finite-difference uncertainties.

Second, the procedure allows a speed-up of sensitivity analyses by one order of magnitude terms of computation time, while remaining fully parallelizable. The approach is demonstrated for a homogeneous (0D) reactor with different complex reaction mechanisms including several reaction types using Cantera.

Large-scale quasi-DNS of mixed-mode turbulent combustion

Thorsten Zirwes (*Karlsruhe Institute of Technology, Germany*)

17:30

Feichi Zhang (*Karlsruhe Institute of Technology, Germany*)

Peter Habisreuther (*Karlsruhe Institute of Technology, Germany*)

Henning Bockhorn (*Karlsruhe Institute of Technology, Germany*)

Dimosthenis Trimis (*Karlsruhe Institute of Technology, Germany*)

In technical combustion devices, fuel and oxidizer are often not perfectly mixed. Therefore, the combustion exhibits both regions with premixed and non-premixed modes. Because of this, many combustion models fail to predict properties of these mixed-mode flames correctly. In this work, a quasi-DNS of the experimentally investigated "Sydney" burner in configuration FJ200-5GP-Lr75-57[1] was performed. It consists of a retractable inner fuel pipe, an annular oxidizer pipe and a surrounding hot pilot flow. The simulation was performed in three steps: 1) A precursor highly-resolved LES for the flow in the fuel and oxidizer pipes to initialize 2) a non-reactive quasi-DNS for the partial mixing of methane and air and 3) a reactive-quasi DNS of the hot pilot igniting the partially premixed methane/air flame downstream.

Both quasi-DNS from step 2) and 3) are performed on numerical grids with 150 million cells each, with a smallest grid size of 5 μm . The quasi-DNS include detailed molecular diffusion coefficients for each chemical species based on rigorous kinetic gas theory and the Hirschfelder-Curtiss approximation. For the chemical reaction rates, finite rate chemistry from a complex reaction mechanism by Lu et al.[2] was applied consisting of 19 physical species and 11 quasi-steady state species. The temporal discretization is implicit and second order in time. For the spatial discretization, a fourth order interpolation scheme with low numerical dissipation is used. The simulation has been performed on the German national supercomputer "Hazel Hen" on up to 28,800 CPU cores with a custom chemistry implementation which increases the performances of reaction rate computations[3].

The discretization schemes have been validated in terms of their numerical dissipation with the well-known Taylor-Green-Vortex. The grid resolution has been validated by comparing subgrid

viscosities that would be predicted by LES models with the molecular viscosity. Finally, the results of the simulations are validated by comparing with experimental data. Time averaged and RMS profiles as well as instantaneous scatter data of temperature and species concentrations at fixed axial positions in the flame show good agreement. The results of the simulations enable to study the transition between premixed and non-premixed combustion regimes in great detail, e.g. by conditioning quantities of interest to the flame index as marker for the different combustion modes.

[1] R. Barlow et al. *Combustion and Flame* 162 (2015) 3516-3540.

[2] T. Lu et al. *Flame* 154 (2008) 761-774.

[3] T. Zirwes et al. *High Performance Computing in Science and Engineering '17*, 2017.

Hierarchical parcel swapping: an efficient mixing model for turbulent reactive flows

Tommy Starick (*BTU Cottbus-Senftenberg, Germany*)

17:50

Heiko Schmidt (*BTU Cottbus-Senftenberg, Germany*)

Turbulent reactive flow simulations are challenging since the flow is characterised by a wide range of length and time scales, which yields high resolution requirements. The computational cost of Direct Numerical Simulations (DNS) that resolve all scales rises with at least the cube of the Reynolds number and is therefore not feasible for engineering applications. Large Eddy Simulations (LES) overcome this limitation by only resolving the large scale effects and modelling the subgrid scale mixing and reaction processes. Hereby, the key challenge is to develop an accurate subgrid mixing model.

Hierarchical Parcel Swapping (HiPS) presents a computationally efficient and novel mixing model [1,2]. In HiPS, the flow domain is interpreted as a binary tree. Every level of the tree corresponds to a length scale. The effects of turbulent advection are represented by stochastic swaps of subtrees at rates determined by turbulent time scales. The mixing of adjacent fluid parcels is done at rates consistent with the prevailing diffusion time scales.

Reactive processes increase the complexity through multiple scalars, which may have different Schmidt numbers. In this work, we demonstrate an extension of the model for variable Schmidt numbers. Results are shown for simple reaction mechanisms at varying Schmidt and Reynolds numbers.

References

[1] A. R. Kerstein, Hierarchical Parcel Swapping Representation of Turbulent Mixing. Part 1. Formulation and Scaling Properties, *Journal of Statistical Physics* (2013).

[2] A. R. Kerstein, Hierarchical parcel-swapping representation of turbulent mixing. Part 2. Application to channel flow, *Journal of Fluid Mechanics* (2014).

Towards an understanding of finite-difference truncation errors through the lens of sparse regression

Ludger Paehler (*Technical University of Munich, Germany*)

18:10

Stephan Thaler (*Technical University of Munich, Germany*)

Nikolaus A. Adams (*Technical University of Munich, Germany*)

When modelling paradigms such as Reynolds-averaged Navier-Stokes approaches and explicit Large-Eddy Simulations (LES) fail at the simulation of complex turbulent flows due to temporal, or spatial scales, or interference of the non-linear truncation error with the subgrid-scale model we have to resort to implicit modelling schemes. Implicit LES utilizes the local truncation error of numerical schemes to model the subgrid-scales. As central as the modified differential equation analysis (MDEA) is to this construction process as arduous can this procedure become when

more complex configurations are being considered. We learn the local truncation error using recent advances in data-driven discovery of Partial Differential Equations (PDEs). For this we use the paradigm of sparse regression, as presented by Kutz and Brunton. Finite-difference schemes offer us the perfect environment for proof of concept applications as we can utilize series expansions to derive the modified differential equations (MDEs). In the current talk we will present an outlook using the linear advection equation, discretized with Forward-Time Backward-Space (FTBS), and the Burgers equation with the Mac-Cormack predictor-corrector scheme. Reducing the multicollinearity of terms used by the sparse regression scheme and using 8th order accurate finite-difference stencils we are able to showcase high accuracy predictions in low noise environments. This underlines the approaches' promise for the analysis and optimisation of discretization schemes.

S10.02 | Turbulence and reactive flows

Date: February 21, 2019
Room: HS 03

08:30-10:30

Phase-field simulations of turbulent two-phase flows

Marc Avila (*University of Bremen, Germany*)

08:30

Baofang Song (*University of Bremen, Germany, Tianjin University, China*)

Carlos Plana (*University of Bremen, Germany*)

Jose M. Lopez (*IST Austria, Austria*)

Alberto Vela Martin (*Universidad Politecnica de Madrid, Spain*)

Phase-field methods have long been used to model the flow of immiscible fluids. Their ability to naturally capture interface topological changes is well established and makes them suitable for the simulation of turbulent two-phase flows, in which droplet breakup and merging occur stochastically in space and time. However, phase-field models feature a model parameter, the mobility, whose value is unknown a priori. Incorrect choices of the mobility lead to wrong interfacial physics, which has hindered the widespread use of phase-field methods. Recently, a physically consistent prescription for the mobility as a function of the interface thickness was derived analytically by Magaletti et al., *J. Fluid Mech.*, vol. 714, pp. 95-126, 2013. Here we investigate numerically their prescription and show its robustness with direct numerical simulations of turbulent two-phase pipe flow with up to one billion grid points. Based on these simulations and other simulations performed for a triply periodic box, the physical mechanisms of droplet breakup in isotropic and wall-bounded turbulent flows will be also discussed. Our results demonstrate the ability of the phase-field method to accurately deal with non-Cartesian geometry, strong advection, turbulent velocity fluctuations and large density and viscosity contrasts.

Direct numerical simulation of flow over rough walls

Pourya Forooghi (*Karlsruhe Institute of Technology, Germany*)

09:10

Alexander Stroh (*Karlsruhe Institute of Technology, Germany*)

Bettina Frohnepfel (*Karlsruhe Institute of Technology, Germany*)

Surface roughness plays an important role in a variety of industrial applications, including gas turbines, internal combustion engines, marine transport and aviation, as well as meteorological applications. Direct Numerical Simulation (DNS) is a strong tool for the study of turbulent flows, where the complexity of near-wall measurements in the experimental approach can be avoided. However, due to the need to capture not only all the flow scales but also the details of

the roughness geometry, DNS over rough walls is particularly challenging and computationally expensive. In this work DNS of flow in rough channels is reported, in which the detailed roughness geometry is reproduced using an Immersed Boundary Method (IBM).

A variety of simulations with different roughness geometries are run in order to understand, firstly, the physics of rough wall-bounded turbulence, and secondly, the effects of roughness geometry, in particular that of roughness density, on the roughness-induced skin friction and the physics of turbulent flow. The results shed light, among others, on the possibility of extracting a universal correlation for equivalent sand-grain roughness size as a function of roughness geometry in the fully rough regime. The channel simulations are carried out in a box domain with periodic boundary conditions in the streamwise and spanwise directions at friction Reynolds numbers up to 500.

Turbulence measurements in high-speed flows with a new Stereo-Dual-PIV system

Anne-Marie Schreyer (*RWTH Aachen University, Germany*)

09:30

Imke Janssen (*RWTH Aachen University, Germany*)

We developed a new Stereo-Dual-particle image velocimetry (Stereo-Dual-PIV) system for turbulence measurements in complex high-speed flows and present first measurement results. The system was primarily designed for analyses of shock wave/turbulent boundary layer interactions (SWTBLI) with separation, a type of flow with major impact and relevance for numerous aerospace-transportation and -propulsion applications. These highly three dimensional flows impose demanding requirements on measurement systems: the range of characteristic frequencies that need to be resolved is large ($O(100 \text{ Hz}-100 \text{ kHz})$), and high spatial and temporal resolutions are necessary for measurements of turbulent quantities in wall-bound flows. To be able to analyze space-time links across the interaction, which is required to better understand the underlying mechanisms in the flow, the field of view should allow simultaneous measurements in the entire flow field. Furthermore, a high laser-pulse energy is needed to provide sufficient illumination for the small tracer particles required in high-speed flows. Existing high-speed PIV systems cannot provide the required temporal and spatial resolutions at the same time.

Our system therefore pursues a carefully synchronized multi-frame approach: two Stereo-PIV systems, each of them delivering all three components of the velocity vector in the measurement plane, are arranged such that they observe the exact same field of view. They thus deliver two sets of PIV-image pairs at a preselected, arbitrarily small temporal delay, making temporal information and thus also spectral information available. The setup includes two double-pulse PIV lasers and four 11MPixel CCD cameras with a 4008 x 2672 pixel sensor, giving access to spectral content without compromising the spatial resolution and data quality. High-accuracy color-based image-separation is applied, using two lasers of slightly different wavelengths together with color filters in front of the cameras. Both lasers have an equally large pulse energy (200 mJ/pulse). The lasers thus have very similar characteristics and generate light sheets with similar properties, so that both systems achieve the same high signal-to-noise ratio.

Measurements at a Mach number of $M=2.5$ are performed in the trisonic wind tunnel at the Aerodynamic Institute of RWTH Aachen University. First measurements in a supersonic shock wave / turbulent boundary-layer interaction will be presented, validating the system against a standard planar PIV-system and presenting the turbulence behavior of all three components of the velocity vectors across the interaction.

Harmonic and pulsatile flow in an aortic aneurysm model: experiments and simulations

Maximilian Christof Bopp (*Technische Universität Darmstadt, Germany*) 09:50
Sebastian Wegt (*Technische Universität Darmstadt, Germany*)
Cameron Tropea (*Technische Universität Darmstadt, Germany*)
Suad Jakirlic (*Technische Universität Darmstadt, Germany*)
Andreas Bauer (*Technische Universität Darmstadt, Germany*)
Nina Shokina (*University of Freiburg, Germany*)
Axel Krafft (*University of Freiburg, Germany*)
Juergen Henning (*University of Freiburg, Germany*)

An ongoing interest in medicine is to prevent cardiovascular diseases, one of those being the development of enlargements of the aorta, so-called aortic aneurysms. The goal is to determine indicators which can predict the growth and rupture of such aneurysms. It is well accepted that the vessels are sensitive to the wall shear stress (WSS), which arises due to the friction of blood flow on the vessel wall. These circumstances motivated the present work, focussing on numerical simulations and experiments of the harmonic and physiologically pulsatile flow in an aortic aneurysm configuration. In the latter case the flow rate variation in time follows closely a realistic physiological blood circulation pulse as encountered in a human aorta. The Reynolds number range considered indicates transitional and low-intensity turbulent flow regimes. The prime objective of the study is the estimation of the time-resolved wall shear stress, representing a parameter of importance for risk estimation of aorta aneurysm rupture. Experimental investigations have been performed by using both Laser Doppler Velocimetry (LDV) and Magnetic Resonance Velocimetry (MRV). MRV provides three-dimensional, three-component velocity fields, which serve as a basis for the wall shear stress estimation. Accompanying numerical simulations employ three different turbulence models - baseline, transition-sensitive and eddy-resolving, all based on a near-wall second moment closure formulation. In accordance with the relatively low Reynolds number range, pure laminar computations have also been performed. The model equations are implemented into the finite-volume-based open source toolbox OpenFOAM®[®], with which all present simulations are performed. Initially, investigations of a stationary flow in a similar Reynolds number range have been performed.

Acknowledgements. The financial support of the German Research Foundation (DFG) (Grant number TR 194/56-1) is gratefully acknowledged. The authors would like to thank the Lichtenberg HPC at TU Darmstadt for the computing time.

S10.03 | Turbulence and reactive flows

Date: February 21, 2019

14:00-16:00

Room: HS 03

A new approach to simulate confined, premixed and slow combustion

Clemens Gößnitzer (*TU Wien, Austria*) 14:00
Herbert Steinrück (*TU Wien, Austria*)

We will present a new solution method in the context of laminar, premixed and slow combustion inside closed geometries. The flame front is treated as a gasdynamic discontinuity along which heat is instantaneously released. We use Markstein's model for the laminar burning velocity. We neglect heat conduction and friction, and the boundaries are adiabatic. By assuming that the combustion is slow, we can expand all equations with respect to a small reference Mach number.

The asymptotic analysis shows that the leading-order pressure is time-dependent only. Thus, the divergence of the velocity is also a function of time only. By splitting the velocity in an irrotational and solenoidal part, we take advantage of the special structure of the problem. The flame front is tracked by marker points. To fulfil the condition for the jump of normal velocity at the interface, a singular volumetric source is prescribed, using the concept of panel methods known from aerodynamic flows. The irrotational part of the velocity field is obtained by solving a Poisson equation with a right-hand side that only depends on time. The divergence-free part of the velocity field is obtained by solving the vorticity transport equation and a Poisson equation with a right-hand side equal to the vorticity. This is done using a discrete Fourier series approach. Since each material fluid element conserves its entropy – except when crossing the flame front – we use a combination of moving and fixed meshes: The vorticity transport equation is solved on Lagrangian mesh points which also keep track of the entropy. Now, the vorticity is interpolated by Fourier transformation to the fixed mesh, and the Poisson equation is solved. Here, we do not need to consider any boundary conditions since they are fulfilled solely by the irrotational part of the velocity field. Our solution approach works for two-dimensional and three-dimensional, rotational symmetric geometries. The results show good agreement between simulation and experiment.

What can we learn from information-entropy about turbulence and Large-Eddy Simulation?

Linus Engelmann (*University of Duisburg-Essen, Germany*)

14:20

Irenäus Wlokas (*University of Duisburg-Essen, Germany*)

Andreas Markus Kempf (*University of Duisburg-Essen, Germany*)

The Shannon entropy is a rigorous measure of information that can be used to evaluate the properties of information in turbulent flows. In this study, the behavior of the Shannon entropy is investigated for LES of an incompressible turbulent channel flow based on the classical DNS of Moser et. al., and the Lorenz-attractor as a simplified model for turbulence. We then try to examine if and how the Shannon entropy can lead to useful insights into turbulence and quality of simulation. The Shannon entropy is calculated based on binning and probability mass functions of the velocity vector components. For the Lorenz-Attractor, its velocities are obtained along the trajectory and Shannon entropy is calculated. Its behavior is interpreted by comparison to other statistical measures, such as standard deviation. For the channel flow, Shannon entropy is calculated from the velocity fluctuation fields and is compared to the turbulent kinetic energy. The quality and resolution of the LES calculations on different grids has been evaluated against DNS results. The Shannon entropy is calculated for velocities and the turbulent viscosity to observe how it behaves and how it related to the simulation quality and grid resolution. The Shannon entropy of velocity fluctuations was found to fall off at the wall and parallels can be drawn between the entropy and the states of order in the flow. The entropy of the modelled viscosity has been investigated in a similar way and a clear effect of grid resolution has been observed.

Vortex cores as barriers to the diffusion of vorticity in 2D turbulence

Stergios Katsanoulis (*ETH Zürich, Switzerland*)

14:40

Mohammad Farazmand (*Massachusetts Institute of Technology, USA*)

George Haller (*ETH Zürich, Switzerland*)

Recent advancements have allowed for diffusion barriers to be identified as material surfaces that inhibit the diffusion of passive scalars more than neighboring surfaces do. The objective (observer-independent) identification of such surfaces has recently been extended to uncover

the material skeletons of diffusive tracer patterns in compressible flows. According to this new formulation, barriers to the diffusion of vorticity are constructed with and without constraining them on a specific initial vorticity distribution. Here, we describe a computational algorithm based on these new results. The algorithm offers a fully automated detection of conservative, constrained and unconstrained diffusive barriers without reliance on user input or fine-tuning of parameters, as other coherent-structure-detection algorithms typically do. We also introduce a publicly available Matlab graphical user interface (GUI) that implements all these results for general, two-dimensional unsteady flow data. We conclude by demonstrating the use of this GUI on a 2D decaying turbulence example.

Lagrangian perspectives on turbulent superstructures in Rayleigh-Bénard convection

Christiane Schneide (*Leuphana Universität Lüneburg, Germany*)

15:00

Amrish Pandey (*Technische Universität Ilmenau, Germany*)

Anna Klünker (*Leuphana Universität Lüneburg, Germany*)

Kathrin Padberg-Gehle (*Leuphana Universität Lüneburg, Germany*)

Jörg Schumacher (*Technische Universität Ilmenau, Germany*)

We analyze large-scale patterns in three-dimensional turbulent convection in a horizontally extended square convection cell by Lagrangian particle trajectories calculated in direct numerical simulations. We consider a simulation run at a Prandtl number $Pr=0.7$, a Rayleigh number $Ra=10^5$, and an aspect ratio $\Gamma=16$. Different Lagrangian computational methods are used to detect these large-scale structures, which are denoted as turbulent superstructures of convection [1].

In a first step, Lagrangian tracer particles are seeded into the simulation domain on a regular mesh with $N=512^2$ points at a plane close to the bottom plate, so well inside the thermal boundary layer. Each individual tracer particle is advected by the flow.

By means of finite-time Lyapunov exponents (FTLE), regions of initial strong separation are identified from the Lagrangian trajectories. The FTLE ridges are signatures of the boundaries between convection rolls. Due to turbulent dispersion this heuristic diagnostic only gives insightful results on very short time scales.

On time scales comparable to the characteristic time of the turbulent superstructures, a spectral clustering approach [2] applied to the Lagrangian trajectories turns out to be successful in detecting large-scale structures. These structures are found to agree very well with the Eulerian superstructures and appear to be bounded by regions of strong separation as measured by the FTLE field.

Longer time periods beyond the characteristic time require a change of the analysis method to a density-based trajectory clustering by means of time-averaged Lagrangian pseudo-trajectories. A small coherent subset of the pseudo-trajectories is obtained in this way consisting of those Lagrangian particles that are trapped for long times in the core of the superstructure circulation rolls and are thus not subject to ongoing turbulent dispersion.

Finally, whereas the FTLE and clustering studies as carried out in [1] focus on the emergence of the superstructures, we also study turbulent trajectories at later times in the simulation. To identify the superstructure circulation roles in terms of almost-invariant flow regions we apply a transfer-operator numerical approach [3]. Here, the superstructures are approximated based on the leading eigenvectors of a stochastic matrix that describes the transition probabilities of the particles between different regions in the convection cell.

References:

- [1] C. Schneide, A. Pandey, K. Padberg-Gehle, J. Schumacher, Phys. Rev. Fluids, accepted (2018).
- [2] A. Hadjighasem, D. Karrasch, H. Teramoto, G. Haller, Phys. Rev. E 93, 063107 (2016).

[3] M. Dellnitz, O. Junge, SIAM J. Numer Anal 36, 491-515 (1999).

RANS-type turbulence modelling using lie-symmetries

Dario Klingenberg (*TU Darmstadt, Germany*)

15:20

Martin Oberlack (*TU Darmstadt, Germany*)

We present a new turbulence modeling framework based on recent developments in the theoretical understanding of turbulent statistics. The work relies heavily on the mathematical theory of Lie-symmetries. Symmetries are defined as transformations that leave equations form invariant. For any given system of equations, it is possible to calculate all symmetries admitted by the system. The symmetries of equations used to describe physical processes often encode important physical principles implicitly contained in the equations such as Galilean invariance. In fact, many equations, including the Euler equations, are uniquely defined by the symmetries they admit if the highest order of derivatives is given. This makes symmetries an extremely useful tool for any modeling process. One can calculate the symmetries of the system for which a reduced model is wanted, and then generate model equations from a specifically chosen subset of symmetries. This leads to a model that is capable of very accurately emulating the behavior of the exact system. In turbulence research, the mathematical notion of symmetries is rarely applied directly, however, many classical concepts of turbulence modeling make use of intuitively found symmetries of the Navier-Stokes equations. E.g., the concept of invariant modeling states a number of conditions that have to be fulfilled by any turbulence model. It can be shown that fulfilling these conditions is essentially equivalent to incorporating all Navier-Stokes symmetries. As all modern turbulence models fulfill the conditions of invariant modeling, i.e they also fulfill all Navier-Stokes symmetries. However, it was recently discovered that the infinite hierarchy of statistical moment equations derived from Navier-Stokes equations contains additional symmetries. These symmetries are intimately connected with Non-Gaussianity and intermittency of turbulent statistics. As turbulence models constitute a statistical description of turbulent flows, we propose that turbulence model equations should contain these symmetries. However, the authors are not aware of any turbulence model that generally fulfills these symmetries. As it turns out to be very challenging to include these symmetries in a model, a new modeling strategy is presented here. Finally, a possible set of model equations is derived using this strategy. The new model can be expected to predict turbulent flow much more reliably, as it naturally incorporates important physics about the statistical behavior of turbulence.

Acknowledgement

The work of Dario Klingenberg is supported by the Excellence Initiative of the German Federal and State Governments and the Graduate School of Computational Engineering at Technical University Darmstadt.

S10.04 | Turbulence and reactive flows

Date: February 21, 2019

17:40-18:40

Room: HS 03

Coherent vortex structure investigation behind the axial fan impeller in pipe

Djordje S. Cantrak (*University of Belgrade, Serbia*)

17:40

Novica Z. Jankovic (*University of Belgrade, Serbia*)

Milos S. Nedeljkovic (*University of Belgrade, Serbia*)

Investigation of the coherent vortex structure in pipe on the axial fan pressure side is reported in this paper. Axial fan has outer diameter 0.399 m, while pipe inner diameter is approximately 0.4 m. The axial fan generates Rankine vortex, which is a combination of the forced vortex, surrounded by a free vortex. Experiments were conducted by use of the one-component laser Doppler anemometry (LDA) and stereo particle image velocimetry (SPIV) systems. In addition, some flow visualization techniques were employed in the turbulent swirl flow investigation. All three velocities (axial, radial and circumferential) were subsequently measured by use of the LDA system. SPIV revealed vortex structure in the cross-section region of approximately 180 mm x 120 mm, while in the vertical meridian section with dimensions approximately 130 mm x 80 mm. All these results are consistent with those presented in previous papers. Here is the focus on the coherent vortex structure.

Obtained experimental results reveal Rankine vortex structure with its four flow regions: vortex core with solid body characteristics, shear layer characterized with the maximum circumferential velocity, sound flow region with constant circulation distribution and the boundary layer region. Levels of turbulence, as well as statistical moments of the higher order for all three velocities are calculated. It was shown that turbulence levels for all three velocity components have the highest values in the vortex core and shear layer regions. All velocities and statistical values distributions are not uniform. It was shown that turbulence anisotropy occurs, as well as that the flatness factor for circumferential velocity in the vortex core region have shown wide spectrum of circumferential velocity fluctuations.

Normalized time autocorrelation functions for circumferential fluctuating velocity in the points in the sound flow region revealed that the correlation coefficients variations were significant, what indicated high frequency circumferential velocity components. On the contrary, correlation curves in the vortex core and shear layer regions revealed dominant role of the low frequency fluctuations. The maximum values of the time integral scale are reached in the vortex core region, what indicated great vortex structures. In addition, vortex core existence and dynamics were analyzed by observing total velocity minima positions and employed statistics. It was shown that most of the time minima occur in the pipe axis vicinity, what is consistent with the turbulent swirl flow characteristics and the existence of the coherent vortex structure.

Reduction of fuel consumption of small gas turbines at idling under combined operation with adjustable compressor inlet and turbine outlet guide vanes

Uwe Borchert (*Fluidenergiemaschinen und Energieanlagen, Germany*)

18:00

Like all heat engines, gas turbines work with reduced efficiency when their partial load is decreased. Compared to their maximum power, gas turbines also consume considerably more fuel during idling than other combustion engines. For the experimental verification of the effect of adjustable compressor inlet guide vanes combined with adjustable turbine outlet guide vanes on the fuel consumption at idling, an 8 kW test gas turbine was designed and built up.

The data of the experiments with the test gas turbine was compared with experimental data acquired by the author from another gas turbine. Additionally, experimental data was compared with external data of other heat engines. It was found that the test gas turbine consumed about 10% less fuel at idling due to only adjusting the compressor inlet guide vanes than with full open compressor inlet.

In addition, the combined adjustment of the guide vanes at the compressor inlet and the turbine outlet resulted in an additional reduction of the fuel consumption at idling by 0.25%. However, the results also clearly show that the additional reduction of the fuel consumption can be achieved only at low idle speed range.

Using the newly introduced dimensionless KRUSCHIK number, the test gas turbine, two series gas turbines and an internal combustion engine was compared in terms of their required heat supply at idling.

Numerical approaches for the simulation of the yeast distribution in a fermentation tank

Daniel Klemmt (*University of Applied Sciences Stralsund, Germany*)

18:20

Heiko Meironke (*University of Applied Sciences Stralsund, Germany*)

In the context of investigations of real multiphase flows, the university has its own 350 litre fermentation tank with comprehensive acoustic flow and temperature measurement technology for the systematic investigation, of the influence of the fermentation activity, distribution of yeast and occurring convection phenomena.

Due to the many problems with the optical and acoustic measurement in a real fermenting fluid the numerical simulation was already used in earlier publications. Models for the simulation of the natural convection flow in a fermentation tank and, in a second step, the superposition of the natural convection by gas bubbles have already been presented in the last GAMM Annual Meeting 2018.

Based on these results, this paper examines the simulation of yeast using the Euler-Lagrange model. The aim is to extend the existing simulation, which is based on the Eulerian-Eulerian time-averaged model and to validate it with measurements from real experiments. The main focus of this study is on the investigation of different approaches to particle interactions and their effects.

Starting point is the Dense Discrete Phase Model (DDPM), which is based on the Kinetic Theory of Granular Flow Model (KTGF) or Discrete Element Method Collision Model (DEM). Especially the physical interaction models, for example the lift force, virtual mass force and collision models, play an important role. These fundamental studies must be conducted because the behaviour of the real yeast is much more complicated than, for example, the interaction of two sand particles. During real fermentation, the yeast increases over time and also combines with other yeast particles. As a result, the proportion of yeast in the process increases and the equivalent particle size also increases due to the combination of the yeast.

The use of user-defined functions is also planned and mandatory, e.g. for the definition of boundary conditions, since a fermentation tank is a closed domain without inlet and outlet.

The goal of this investigation is a numerical simulation of the flow processes in the fermentation tank, based on the Eulerian-Eulerian model with the additional DDPM as realistic as possible, taking into account the natural convection flow and the actual bubble behaviour as well as the yeast distribution.

S11 | Interfacial flows

Organiser: Tatiana Gambaryan-Roismann (*Technische Universität Darmstadt, Germany*)

Rodica Borcia (*Brandenburg University of Technology (BTU) Cottbus – Senftenberg, Germany*)

S11.01 | Interfacial flows

Date: February 19, 2019

08:30-10:30

Room: HS 02

Bubble-particles collision and attachment in laminar and turbulent flows

A.-E. Sommer (*Helmholtz-Zentrum Dresden-Rossendorf, Germany*)

08:30

M. Eftekhari (*Helmholtz-Zentrum Dresden-Rossendorf, Germany*)

A. Javadi (*Helmholtz-Zentrum Dresden-Rossendorf, Germany, TU Dresden, Germany*)

S. Heitkam (*Helmholtz-Zentrum Dresden-Rossendorf, Germany, TU Dresden, Germany*)

K. Schwarzenberger (*Helmholtz-Zentrum Dresden-Rossendorf, Germany*)

Kerstin Eckert (*Helmholtz-Zentrum Dresden-Rossendorf, Germany, TU Dresden, Germany*)

Bubble-particles collisions and attachment in flows refer to a challenging multi-scale process, comprising length scales from $O(m)$, where energy is injected into the flow, towards $O(10^{-9} m)$ on which the thin film between bubble and particles ruptures. Bubble-particles collisions are not only interesting from the fundamental point of view but they also possess high relevance in large-scale separation processes in industry. The most prominent case is the so-called froth flotation being a basic technology in mineral processing. In this process, hydrophobized valuable particles attach to the interface of gas bubbles rising in a suspension of valuables and gangue mineral particles. The success of the process, expressed in terms of the flotation recovery depends on both the surface chemistry used for the hydrophobization of the particles and the hydrodynamics for an encounter between bubble and particle.

In the first part of the talk, the present understanding of bubble-particles collisions and attachment in both laminar and turbulent flows is reviewed and open issues are addressed. In the second part of the talk we report on recent experimental work in our group devoted to the study of bubble-particles on both meso- and microscale.

On the meso-scale we focus on the measurement of the collision probability of particles with low Stokes number at the bubble surface using 4D particle tracking velocimetry. Here, the particle and bubble trajectories were measured simultaneously with a high temporal (1000 fps) and spatial resolution (0.03 mm/pixels). An algorithm was developed to evaluate the flotation recovery based on the collision and attachment probability [1] of hydrophobic fluorescent polystyrene particles of different sizes. In the case of fine particles, the results show that a significant number of collision events takes place not only at the fore pole of the bubble but also at the rear pole of the bubble due to a higher acceleration within the vortices in the wake. On the microscale, a particle-laden flow impinging a stagnant bubble is studied using Micro-PIV. Here, particular emphasis is laid on a better understanding of the change from free-slip (mobile interface) towards the no-slip boundary condition (immobile interface) which is known to decrease the collision probability.

[1] AE Sommer, M Nikpay, S Heitkam, M Rudolph, K Eckert, *Minerals Engineering* 124, 116-122 (2018)

Oscillating hydrogen bubbles at microelectrodes

Aleksandr Bashkatov (*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany*) 09:10
Xuegeng Yang (*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany*)
Sahil Hossain (*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany*)
Gerd Mutschke (*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany*)
Kerstin Eckert (*Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany, Technische Universität Dresden, Germany*)

Hydrogen produced via water electrolysis, which is powered by renewable energy, is an important energy carrier which may contribute to bridge the storage problem. However, the efficiency of alkaline water electrolyzers is not yet satisfying. Major reasons are the blockage of the active electrode area and the increase the ohmic resistance by the gas bubbles produced.

A deeper understanding of the mechanism of hydrogen bubble evolution therefore may provide additional opportunities to control and enhance the process. Microelectrodes which allow the inspection of single hydrogen bubble evolution are an interesting tool for that purpose [1].

Shadowgraphy and micro-PIV techniques, coupled to measurements of the electric current under potentiostatic mode at a 100 μm Pt electrode led to observation of a novel dynamic phenomenon. This consists in an oscillatory behavior of the hydrogen bubbles at the electrode, which depends on the applied potential and the concentration of the acidic electrolyte. With increasing potential a transition from periodic upward and downward movements of the bubble towards bubble shape oscillations is observed. This phenomenon is connected with the formation of a carpet of a small bubbles at the foot of the growing bubble and includes an oscillatory form of the Marangoni convection recently found on hydrogen bubbles [2]. Two possible candidates for the driving mechanism of the oscillations are discussed.

References:

[1] Yang, Xuegeng, et al. Dynamics of single hydrogen bubbles at a platinum microelectrode. *Langmuir* 31.29 (2015): 8184-8193.

[2] Yang, Xuegeng, et al. Marangoni convection at electrogenerated hydrogen bubbles. *Physical Chemistry Chemical Physics* 20.17 (2018): 11542-11548.

Numerical investigation of simultaneous multi-bubble collapse scenarios with varying initial size

Aleksandr Lunkov (*Technical University of Munich, Germany*) 09:30
Stefan Adami (*Technical University of Munich, Germany*)
Nikolaus A. Adams (*Technical University of Munich, Germany*)

It is known that fluid dynamics processes occurring during medical operations such as extracorporeal shock wave lithotripsy can cause benign tissue damage. This damage is a consequence of the high-speed jets impact which are caused by asymmetric shock-induced gas-bubble collapses in a liquid medium. On the other hand, this mechanism can be used to perforate cell membranes for efficient high-precision drug delivery. Unfortunately, these phenomena are yet not well-understood quantitatively and experimental measurements are very complex as the time and spatial scales of the collapse dynamics are extremely small. Thus, the numerical study of liquid jets and bubble collapses near tissue is carried out in this work. For the computational investigation of this problem, we consider a viscous fluid as a surrogate tissue model. Numerical simulations are conducted using a multi-material sharp-interface method. We consider the setup with two bubbles which are located at the same distance to the tissue-like fluid surface and vary the size of one of them. During the simulation, the bubbles collapse under the influence of a

shock wave. These collapses are followed by the jet formation in the direction of the surface. We investigate the effect of the mutual impact of the bubble collapses on the post-collapse jets characteristics, the penetration depth, as well as the width and the shape of holes caused by the jets. The obtained information can help to estimate the impact of the procedure on the tissue under different operating conditions in the mentioned biomedical applications.

Numerical investigations of the hydrodynamics and oxygen mass-transfer in aerated tanks

Ann Kathrin Höffmann (*TU Dortmund, Germany*)

09:50

Peter Ehrhard (*TU Dortmund, Germany*)

Aeration tanks represent a major energy consumer in municipal wastewater-treatment plants. To increase their efficiency, numerical investigations are conducted to capture the hydrodynamics, the mass transfer, and the biochemical reactions in the aeration tank. Numerical computations offer the opportunity to test system configurations and operating modes without cost-intensive reconstruction work.

The present work concentrates on numerical investigations of the hydrodynamics of rising air bubbles in the activated sludge. In an aeration tank of pilot-plant scale, the bubble rise, the oxygen mass-transfer into the activated sludge, and the biochemical reactions are computed. To validate the numerical model, the oxygen concentration, the ammonium concentration and the nitrate concentration at the outlet are discussed, using also experimental results. Furthermore, the operating mode and the system configuration of the pilot-plant are varied and evaluated with respect to the oxygen demand. These computations, at the end, enable to a statement about the energy efficiency.

On the influence of strain hardening on a rising bubble

Stefan Descher (*University of Kassel, Germany*)

10:10

Olaf Wünsch (*University of Kassel, Germany*)

The phenomena occurring for rising bubbles in non-Newtonian fluids are well investigated, both experimentally and numerically. Viscoelastic fluids, a subclass of non-Newtonian fluids, usually show a variety of effects. Those are shear thinning and strain thickening behavior, normal stress differences and stress relaxation. Thus during the interpretation of results the question comes up, which property causes the shape the bubble takes during rising. In general, it is a combination of all, since the flow around a rising bubble contains shear and extensional flow regimes. Therefore a clear assignment is not possible.

For that reason, in this contribution, a model based on the invariants of the strain rate tensor as introduced in [1] is used. It enables to model a viscous fluid that is Newtonian in its shear behavior, strain hardening and has no normal stress differences. Studies are performed for a three-dimensional rising bubble benchmark [2] using OpenFOAM. Results for different Reynolds and Eötvös number combinations are presented for a varying dimensionless number that considers the strain behavior.

[1] G. Böhme: Strömungsmechanik nichtnewtonscher Fluide. Teubner, 2000 , 2nd edition.

[2] J. Adelsberger, P. Esser, M. Griebel, S. Groß, M. Klitz, and A. Rüttgers: 3D incompressible two-phase flow benchmark computations for rising droplets. WCCM 11 Proceedings (2014).

S11.02 | Interfacial flows

Date: February 19, 2019

16:30-18:30

Room: HS 02

Interfacial flows described by reduced models

Michael Bestehorn (*BTU Cottbus-Senftenberg, Germany*)

16:30

Instabilities and subsequent non-equilibrium pattern formation is often encountered in spatially extended systems. If one of the space dimensions is distinguished for physical or geometrical reasons, dimension-reduced models may be derived successfully by integrating out that dimension. Here we consider (thin) liquid films on a horizontal substrate where the particular dimension is the vertical one. In fluid mechanics, the nowadays called 'Shallow Water Equations' were historically the first dimension-reduced set derived by Adhemar Jean Claude Barre de Saint-Venant already in 1871, allowing for the theoretical and later on numerical linear and nonlinear computations of long surface gravity waves on rivers, lakes or oceans if viscosity can be neglected. Another way of dimension reduction is obtained by enslaving many temporally fast modes by only the few slow modes normally present in the neighborhood of instabilities. The celebrated Swift-Hohenberg equation (Jack Swift and Pierre Hohenberg, 1977) and its extensions derived in the 80ies and 90ies of the last century describes qualitatively well the behavior of several pattern forming convection instabilities also including effects of a free surface. In thin liquid films, normally viscosity is the dominating mechanism and inertia can be neglected (zero Reynolds number limit). Thus, after integrating out the vertical dimension, fluid velocity is enslaved by the film profile and a single 2D equation for the film thickness turns out, as first demonstrated by Agienus Vrij in 1966. However, there are cases even in thin films where the Reynolds number can be large (falling films, mechanically vibrated substrates) and inertia must be kept. This leads to extended thin-film equations where the dynamics of the fluid flow occurs as additional degree of freedom. In this contribution, the situation of parametrically excited films by mechanical vibrations will be studied in more detail. Linear stability as well as nonlinear results of the reduced model will be presented and compared to findings of the full set of hydrodynamic basic equations. Nonlinear results of the reduced model show interesting new patterns like confined pulses or quasi-periodic geometries.

Horizontal Faraday instability and parametric excitation in a circular channel

Ion Borgia (*BTU Cottbus-Senftenberg, Germany*)

17:10

Rodica Borgia (*BTU Cottbus-Senftenberg, Germany*)

Michael Bestehorn (*BTU Cottbus-Senftenberg, Germany*)

Sebastian Richter (*BTU Cottbus-Senftenberg, Germany*)

Wenchao Xu (*BTU Cottbus-Senftenberg, Germany*)

Uwe Harlander (*BTU Cottbus-Senftenberg, Germany*)

We excite surface waves in a circular channel placed on a rotating table. The tank can rotate with constant velocity and/or can librate. The experiment works in two parameter regimes: high libration amplitudes and small frequencies are used for the generation of traveling surface waves, while smaller amplitudes and higher frequencies are necessary for studying the patterns generated by horizontally excited Faraday waves. For the parametric excitation regime, lower viscosity liquids (pure water) can be used. For an efficient excitation, a wall should be placed in the channel. The horizontal Faraday instability in high viscosities liquids (glycerin-water solutions) can be excited only by the mean of the shearing. The wall is not any more necessary. In this way periodic lateral boundary conditions are assured. The experimental and simulation results will be compared.

Observations of wave patterns affected by sub-surface shear currents

Simen Å. Ellingsen (*Norwegian University of Science and Technology, Norway*)

17:30

Benjamin K. Smeltzer (*Norwegian University of Science and Technology, Norway*)

Eirik Aesoev (*Norwegian University of Science and Technology, Norway*)

Ring waves and ship waves have been known since the dawn of time, and studied since the 19th century. Only in recent years, however, has theoretical predictions appeared of how they would look when propagating upon a sub-surface shear current such as might occur e.g. in river deltas or the wind-swept upper ocean. A number of striking predictions have been made; ring waves become asymmetrical, and ship waves take different opening angles and appearance along vs against the current, and become skewed for motion across the current. Thus Kelvin's classical result that deep-water gravity waves always form an angle of 19.5[deg] no longer holds. Neither of these phenomena exist upon a current of uniform depth dependence, nor have they been previously reported in the literature to have been observed.

We report laboratory observations of sheared ship and ring waves where theoretical predictions are confirmed. Striking qualitative departure from quiescent water patterns are found, and all observations are in excellent qualitative and quantitative agreement with theoretical predictions within the error margins of our first-generation experiment.

The experiments were performed in a purpose-built laboratory at the Norwegian University of Science and Technology wherein controlled surface waves can be created atop a bespoke shear current. Surface waves were measured using a synthetic schlieren method, and the sub-surface velocity profile was measured using particle image velocimetry (PIV).

Beautiful and inherently interesting as these phenomena are, they also have profound real-life consequences. For example, we recently predicted that the presence of shear in the Columbia River mouth would effect a difference of a factor 3 for wave-making resistance on smaller ships sailing upstream vs downstream at the same speed relative to the surface, with obvious consequences for optimal route planning. The effect of shear on wave loads, however, is not accounted for in engineering today. Moreover, wave steepness in the same treacherous waters, often called "the Graveyard of the Pacific" was found to be grossly mispredicted when shear was unaccounted for. Our observations lend further strong support to the reality of these large predicted effects, underlining the necessity to develop predictive tools to account for shear in wave models and wave load calculation.

Thin liquid film formation on hemispherical and conical substrate

Markus Scholle (*Heilbronn University, Germany*)

17:50

Florian Marner (*Heilbronn University, Germany, Durham University, UK*)

Philip H. Gaskell (*Durham University, UK*)

Amy E. Morris (*Durham University, UK*)

The deposition and coating of thin films onto curved rigid substrate, involving displacement of air by a liquid, has numerous applications within the technology sectors but faces two major challenges: (i) control of the local film thickness; (ii) ensuring that the coating remains stable. The work reported here investigates the full coverage of three-dimensional curved geometries, of hemispherical and conical shape, by a continuously fed, gravity-driven, thin liquid layer. The modelling approach adopted utilises a first integral formulation [1,2] of the Navier Stokes equations leading to a variational formulation in the case of steady flow and an advantageous re-formulation of the dynamic boundary condition at the free surface [3]. Asymptotic

analysis, underpinned by the long-wave approximation, enables analytic solutions for the local film thickness and the internal flow to be obtained.

The above new results are placed in context by comparing them with the findings of [4] together with recently acquired new experiments and flow visualisations specific to film flow on conical surfaces [5], prior to the onset of and post instability. In conclusion, a perspective is provided in relation to how the findings form the basis for a corresponding stability analyses to study the onset of unsteady phenomena such as solitary waves and, in the case of incomplete wetting, rivulet formation.

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S11.03 | Interfacial flows

Date: February 20, 2019

08:30-09:30

Room: HS 02

Gradient structures for flows of concentrated suspensions - jamming and free boundaries

Dirk Peschka (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany*) 08:30

Marita Thomas (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany*)

Barbara Wagner (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany*)

Andreas Münch (*University of Oxford, UK*)

In this talk, we will present a two-phase model for the flow of concentrated noncolloidal suspensions. Using gradient flow structures a PDE formulation will be constructed in a systematic way, featuring different coupling mechanisms and driving forces. We will focus on three main aspects: the role of normal pressures, the transition to jamming, the incorporation of free boundaries.

For example, in order to introduce normal pressures into the nonlinearly coupled model, one has to introduce certain nonsmooth dissipative terms. This contribution is essential since the normal pressure is the basis for effective particle transport in a suspension generally known as shear-induced migration.

Particle accumulation in high-Prandtl-number liquid bridges

Ilya Barmak (*TU Wien, Austria*) 08:50

Francesco Romanò (*TU Wien, Austria, University of Michigan, Ann Arbor, Michigan, USA*)

Hendrik C. Kuhlmann (*TU Wien, Austria*)

Particle accumulation in high-Prandtl-number thermocapillary liquid bridges is studied numerically. To that end, high-resolution three-dimensional numerical simulations are carried out for liquid bridges of different length-to-radius aspect ratios for several Reynolds numbers. The considered parameters are above the onset of thermocapillary instabilities, and a three-dimensional hydrothermal wave, which travels in azimuthal direction, is always observed. Therefore, the flow topology can be conveniently analyzed using Poincaré sections in a frame of reference rotating

with the angular velocity of the hydrothermal wave, where the flow is steady and just a single accurate snapshot is needed to investigate the flow topology. The thermocapillary flow under consideration is characterized by much thinner thermal boundary layers than for low-Prandtl liquid bridges studied previously. Therefore, numerical resolution requirements are tighter, in particular, in the region near the free surface, which is of key importance for the particle accumulation phenomenon. High-resolution simulations enable identification with sufficient accuracy of various sets of Kolmogorov-Arnold-Moser (KAM) tori of the flow, which are known to provide templates for particle accumulation structures (PAS). Furthermore, different models of particle motion are investigated for a dilute suspension in order to study the effect of particle inertia, particle-surface and particle-particle interactions. The latter is important during the final stage of the PAS formation when the particle density along the PAS becomes significant.

S11.04 | Interfacial flows

Date: February 20, 2019
Room: HS 02

14:00-16:00

Controlling sliding droplets with optimal contact angle distributions and a phase field model

Henning Bonart (*Technische Universität Berlin, Germany*)

14:00

Christian Kahle (*Technische Universität München, Germany*)

Jens-Uwe Repke (*Technische Universität Berlin, Germany*)

In many process engineering apparatuses and processes, liquid drops move on solid surfaces. Examples are the packing structures in absorption columns, purification and coating processes or multiphase condensers and microreactors. In particular, the interaction between droplet and solid surface is determined by the contact angle. For some time now there have been experimental approaches to utilize a specific contact angle distribution of the surface to influence the speed and the path as well as the wetting of the drops. This allows to set specific residence times of sliding drops on inclined surfaces. In previous work, we improved and implemented a complex model for detailed and energy-consistent simulations of moving contact lines and applied it to sliding droplets. The dynamics of the two-phase flow are described by the Cahn-Hilliard (CH) equation and coupled to the Navier-Stokes (NS) equations. The CH equation models the interface between the fluids with a diffuse interface of positive thickness and describes the distribution of the different fluids by a smooth indicator function. Especially, the CH equation allows the contact line to move naturally on the solid surface due to a diffusive flux across the interface, which is driven by the gradient of a chemical potential. Building on this, we present the structure and first results for the optimal control of droplets on solid surfaces. The static contact angle distribution acts as the control variable and the CHNS model is used to calculate the drop dynamics. As optimization problems, the specification of a desired drop shape, a velocity trajectory and the resulting residence time might be considered.

Phase-field modeling of fluid-structure interaction

Sebastian Aland (*HTW Dresden, Germany*)

14:20

We consider the coupling of a fluid with elastic solid bodies. As opposed to traditional approaches to fluid-structure interaction, we do not describe these domains by a moving grid. Instead, an implicit description by a phase-field function is employed to characterize the evolving domains, which offers some interesting advantages from a modeling point of view. We discuss a simple approach leading to a fully Eulerian two-phase flow problem with an additional elastic stress in

the solid bulk. The approach is validated by comparison to ALE simulations and experiments. Extensions to viscoelastic fluids and membranes are presented along with a recent application to biological cells in flow.

Numerical treatment of interfaces

Dietmar Kroener (*University Freiburg, Germany*)

14:40

In this contribution we will consider moving interfaces and partial differential equation on moving interfaces in different contexts. First we will present the existence, uniqueness and numerical experiments for solutions of nonlinear conservation laws on moving surfaces. In addition to the "hydrodynamical" shocks, geometrically induced shocks will appear. In the second part we study the compressible two phase flow with phase transition on the bases of the Navier-Stokes-Korteweg- and a phasefield model. It turns out that it is extremely important for the numerical schemes of both models that they satisfy a discrete energy inequality to satisfy the second law of thermodynamics. Different numerical experiments will be presented. In the third part we will report on recent research on our experience of the application of the volume of fluid method (VOF) for the resolution of interfaces. The main advantage compared to level set methods is , that the VOF method is mass conserving. We will show different numerical experiments for the movement of droplets on solid walls.

These results have been obtained together with S. Burbulla, D. Diehl, J. Gerstenberger, M. Kränkel, T. Malkmus, T. Müller, M. Nolte, C. Rohde.

An arbitrary Lagrangian-Eulerian formulation for fluid flow on evolving surfaces

Roger A. Sauer (*RWTH Aachen University, Germany*)

15:00

Amaresh Sahu (*UC Berkeley, USA*)

Yannick A. D. Omar (*UC Berkeley, USA*)

Kranthi K. Mandadapu (*UC Berkeley, USA, Lawrence Berkeley National Laboratory, USA*)

Understanding fluid flow on evolving surfaces is essential to understanding fluidic membranes, like soap films and lipid bilayers. Fluidic membranes are numerically challenging because they cannot be described properly by a pure Eulerian or a pure Lagrangian description. This motivates the development of an arbitrary Eulerian-Lagrangian (ALE) formulation for fluid flow on curved and evolving surfaces. The formulation is based on a rigorous surface description in the framework of differential geometry, which provides a general framework to describe fluid surfaces, such as lipid membranes [1]. An arbitrary curvilinear coordinate is introduced that is generally different from an Eulerian and a Lagrangian surface description. Based on this, the ALE equations for the surface velocity, acceleration and density are derived in the general context of curved surfaces. This is then used to propose a computational formulation that allows for an arbitrary mesh update. The strong form and the weak form for this formulation are presented, and their discretization in the framework of nonlinear finite element methods [2] is discussed. Several analytical and computational examples are presented to illustrate the new formulation.

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The role of degenerate mobilities in Cahn-Hilliard models

Marion Dziwnik (*University of Hamburg, Germany*)

15:20

In this talk we elucidate the role and influence of degenerate mobilities in phase field models for interface diffusion dewetting. The equation of interest is the Cahn-Hilliard equation (in two space dimensions) with a polynomial double well free energy and different order-parameter dependent, degenerate mobilities. In contrast to some results found in the literature, a detailed matched asymptotic analysis shows that the sharp interface limit is non-unique, and subtly depends on how degenerate the mobility is. Whilst a quadratic degenerate mobility leads to a sharp interface model where bulk diffusion is present at the same asymptotic order as surface diffusion, higher degenerate mobilities lead to a sharp interface model where bulk diffusion is subdominant. In particular, the corresponding numerical simulations reveal that the type of the degeneracy has a qualitative impact on the evolution: Considering the dewetting process of a thin solid film, the evolution with bi-quadratic degenerate mobility turns out to be more effective for film pinch-off than with quadratic degenerate mobility. The results will be compared and related to other Cahn-Hilliard type models where diffusional mobilities play a decisive role.

Two-phase flow simulations for mold filling on 4D simplex space-time meshes

Violeta Karyofylli (*RWTH Aachen University, Germany*)

15:40

Max von Danwitz (*RWTH Aachen University, Germany*)

Lutz Pauli (*RWTH Aachen University, Germany*)

Marek Behr (*RWTH Aachen University, Germany*)

Mold filling is of great importance for the die-casting and injection molding processes, because many defects of the components may occur during this stage. Therefore, its numerical modeling is crucial for predicting and determining the quality of the produced parts. However, various complicated phenomena (e.g., wetting, heat transfer, non-Newtonian behavior, etc.) emerge while filling compound geometries with complex materials. As a consequence, its numerical simulation is tremendously challenging and requires not only accuracy but also efficiency.

The objective of this presentation is to emphasize how local time-stepping is applied to mold filling cases, by means of space-time finite element discretization. 4D simplex space-time elements, referred to as pentatopes [1], lead to completely unstructured grids with varying levels of resolution both in space and in time. The method used for applying adaptive temporal refinement in the vicinity of melt-air fronts has been already described in [2] with regard to benchmark cases.

The transient, incompressible Navier-Stokes equations describe the two-phase flow during the cavity filling. The molten material entering the mold is assumed to be a temperature-dependent shear-thinning fluid. That being the case, the heat equation is strongly coupled with the Navier-Stokes equations. The level-set method is used to capture the interface, due to its inherent ability to account for severe topological changes [3]. We use a stabilized space-time finite element formulation for discretizing the equations and the stabilization parameter is defined based on the covariant metric tensor, as shown in [4]. Its definition is extended to 4D and allows us to deal with complex anisotropic simplex space-time meshes.

The numerical examples, used for highlighting the novel discretization approach, include benchmark two-phase flow problems with moving contact lines and the filling simulation of different mold cavities, where the wetting plays a significant role in the interaction of the evolving front with the cavity walls.

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S11.05 | Interfacial flows

Date: February 20, 2019

16:30-18:30

Room: HS 02

Effects of fluid rheology and wetting properties on the droplet motion by a shear flow

Beawer Barwari (*Bergische Universität Wuppertal, Germany*)

16:30

Sebastian Burgmann (*Bergische Universität Wuppertal, Germany*)

Artur Bechtold (*Bergische Universität Wuppertal, Germany*)

Martin Rohde (*Bergische Universität Wuppertal, Germany*)

Uwe Janoske (*Bergische Universität Wuppertal, Germany*)

Droplet dynamics play an important role in various technical processes, e.g. in the field of heat transfer or process technology. Condensed droplets or liquid sprays may attach and adhere to the surfaces of the apparatus. In most cases a superposed gas flow is present which influences the stability of the droplet. If a critical velocity of the gas flow is exceeded, the initially adhering droplets become unstable and may move along the surface. Despite numerous studies, the mechanisms of the droplet movement and the phenomenon of dynamic wetting are still insufficiently described and understood, since a systematic investigation of the specific influence of liquid viscosity, surface tension, surface structure and droplet size has not yet been performed in detail. Furthermore, due to the complexity of the topic, the influence of a turbulent flow on wetting phenomena have received only little attention.

The present contribution deals with the experimental investigation of droplet volumes up to 40 μl within a Plexiglas-channel at different flow velocities using transmitted light technique. A number of water-glycerine and water-ethanol solutions are investigated for the droplet to analyze rheology-effects. Droplets are placed on the bottom channel wall with a syringe. The material of the wall can be changed by replacing the wall segment with different substrates. In this study acrylic glass and coated silicon wafers are investigated to analyze the effect of surface tension and structure. The volume flow rate of the channel air flow is defined by a mass flow controller and is linearly increased until the droplet starts to move and is transported downstream. The velocity profile upstream and downstream of the droplet is measured by hot-film anemometry. It was found that the droplet movement can be categorized into different motion patterns depending on the investigated parameters. The critical velocity required for the droplet detachment decreases with the droplet volume. As the glycerine mass fraction increases i.e. the viscosity increases, the critical velocity increases. For all substances, the critical velocities for the coated silicon wafers are below those of acrylic glass due to the increase of hydrophobicity of the substrate. The surface tension of the droplet has no influence on the critical velocity. By using the dimensionless droplet Reynolds number and the Laplace number a global law for the critical velocity for droplet detachment can be found.

Modelling of shear driven drop motion and groove interaction on smooth rigid substrates

Patrick M. Seiler (*Technische Universität Darmstadt, Germany*)

16:50

Ilia V. Roisman (*Technische Universität Darmstadt, Germany*)

Cameron Tropea (*Technische Universität Darmstadt, Germany*)

Predicting the motion of aerodynamically driven drops on smooth rigid substrates is of great interest for many applications. Some examples for fields where such a prediction is valuable are airblast atomization, printing, airframe ice accretion, process engineering as well as vehicle soiling. Nevertheless, only few studies have been published in this field. The present study attempts to mitigate this by introducing two new physical models. The first model allows the prediction of drop motion on substrates due to aerodynamic forces. It relies on the drop volume, gas flow velocity in the vicinity of the drop, surface tension, as well as the contact angle hysteresis of the involved substrates. The second model compliments the description of the drop velocity. Using the widely-known Lambert W. function the interaction between a drop and a groove can be predicted. It allows estimation of how a drop will behave when encountering a groove.

In order to derive these models, experiments in a fully developed turbulent channel flow were conducted. A image processing tool detects the contour of the drop using a subpixel method. Using the quantified properties of the drop, it is possible to calculate the drop velocity. From hot-wire measurements of the velocity gradient at the wall, the local gas flow velocity at half drop height is known. This velocity is referred to as the attack velocity. A relationship between the attack velocity and drop motion velocity is derived. The second set of experiments with a generic groove was performed in the same wind tunnel. The investigated groove had a variable width. The drop velocity, groove width as well as drop volume were varied and observations of the drop behavior will be presented and discussed.

Acknowledgements This work is financially supported by Adam Opel AG as part of a cooperation with TU Darmstadt. The authors express appreciation to F. Werner and P. Klaus of Adam Opel AG, who provided feedback and valuable input for the experiments. The authors also thank T. Ecker for his input on this study. Patrick M. Seiler is also grateful for support through DFG SFB 1194.

A novel two-step model to investigate turbulent gas flows shearing thin liquid films

Achim Bender (*Technische Universität Darmstadt, Germany*)

17:10

Alexander Stroh (*Karlsruher Institut für Technologie, Germany*)

Bettina Frohnepfel (*Karlsruher Institut für Technologie, Germany*)

Peter Stephan (*Technische Universität Darmstadt, Germany*)

Tatiana Gambaryan-Roisman (*Technische Universität Darmstadt, Germany*)

In many industrial applications thin liquid films are sheared by a turbulent gas flow. Diesel and gasoline fuels, for example, are known to form wall films in the cylinder after injection. Deposits, which have a negative influence on the combustion process, can form from those films especially in the vicinity of three-phase contact lines, which appear as a result of the film rupture. This is why it is important to understand the influence of the turbulent gas flow on film stability and evolution.

In this work, we investigate numerically the dynamics of a thin liquid film, which is sheared by a turbulent gas flow. It has been shown previously that even constant shear stress has an influence on film stability. We are interested in the effect of turbulent fluctuations on the film

development. The simulation is carried out in two steps. In the first step a direct numerical simulation (DNS) of a single-phase channel flow of the gas is performed. The shear stress at the lower wall, which varies with position and time is stored and serves as a boundary condition in the liquid flow problem. In the second step a one-sided long-wave simulation of the liquid film is conducted using the previously gathered shear stress data as a boundary condition at the liquid-gas interface. The resulting film evolution is investigated for two different Reynolds numbers of practical relevance and the influence of the fluctuating turbulent shear stress data on the film deformations is studied.

The results show that it is not enough to evaluate the mean velocity of the gas phase to predict the response of the liquid film to the turbulent shear stress. The characteristic size and the time scale of the turbulent fluctuations significantly affect the film dynamics. Furthermore, it is shown that the propagation velocity of the film plays an important role. The maximum amplification of the film disturbances occurs for the cases where the propagation velocity of the turbulent structures is equal to the surface velocity of the liquid film.

Acknowledgements: The authors would like to thank the German Research Foundation DFG for their financial support within the Collaborative Research Centre SFB/TRR 150 "Turbulent, chemical reactive near-wall multiphase flows", subprojects B01 & B02.

This work was performed on the computational resources ForHLR Phase I & II, funded by the Ministry of Science, Research, and the Arts Baden-Württemberg and the German Research Foundation within the framework program bwHPC.

Numerical investigation of the liquid-jet formation during water-hammer experiments

Vladimir Bogdanov (*Technical University of Munich, Germany*)

17:30

Stefan Adami (*Technical University of Munich, Germany*)

Nikolaus A. Adams (*Technical University of Munich, Germany*)

Liquid jets emerging from curved interfaces after shock impact have recently been in the focus of a number of experimental and numerical investigations as they occur as a part of a lot of various medical and industrial applications, such as lithotripsy, needle-free injection or inkjet printing. However, the details of the jetting phenomenon are far from being fully understood due to its complexity. An open question is, e.g., the influence of wetting effects at the contact line of a liquid-filled cylinder that affect the contact angle and curvature of the interface. We perform a numerical analysis of this problem using the results of the experiment of Kiyama et. al. (Kiyama et. al. 2015) as a reference. In their paper, the liquid-jet formation of silicone oil in an impulsively accelerated vertical test tube is studied experimentally. We use the conservative sharp-interface method with adaptive multiresolution and develop a specific contact-angle boundary condition in order to adequately represent interfacial effects. The method is capable to numerically reproduce the jet formation and to capture wetting effects taking place at wall boundaries. Hence, we can investigate the jet development close to solid walls which provides us with an instrument to carry out the numerical studies of numerous applications.

Effect of a rotating magnetic field on the decay of a free-falling metal jet

Tom Kasper (*TU Bergakademie Freiberg, Germany*)

17:50

Rüdiger Schwarze (*TU Bergakademie Freiberg, Germany*)

Additive manufacturing revolutionizes upcoming technologies. Established techniques are e.g. metal laser sintering and selective laser melting. These processes use metal powder as their basic material. The quality of their final product is restricted by significant powder characteristics like size distribution, droplet shapes and composition. [1,2]

In general, metallurgical atomization processes can be used to produce metal powder. An atomization process begins by melting a steel alloy in a furnace. After lifting a stopper rod, liquid steel flows out of a nozzle as a gravity-driven free-falling jet. Furthermore, an additional high-pressure inert gas stream is directed on the melt to atomize it. [3]

One way to enhance the atomization process is the use of a rotating magnetic field (RMF). The main aim of this investigation is to indicate the effect of RMF of a free-falling metal jet. For this purpose, a numerical model was created in the open-source library OpenFOAM. Therefore, the volume of fluid approach was employed to track the free surface of the jet. To describe the turbulence, implicit large eddy simulation was adopted.

The free-falling melt jet is analyzed for different operating conditions. By increasing the RMF, a rotational flow occurs and the flow velocity increases. This effectuates the free-falling jet and can lead to a helix surface or a hollow-cone jet shape. Moreover, the jet disintegrates into ligaments and small droplets can be observed.

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S11.06 | Interfacial flows

Date: February 21, 2019

08:30-10:30

Room: HS 02

Heat transfer modeling of confined bubble evaporation in a microchannel

Sahba Sadir (*Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*)

08:30

Mohammadmahdi Talebi (*University of Freiburg, Germany*)

Peter Woias (*University of Freiburg, Germany*)

Roland Dittmeyer (*Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*)

Bettina Frohnäpfel (*Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*)

Alexander Stroh (*Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*)

High heat dissipation from a small area is an essential focus of future technologies for semiconductor and microelectronic devices. Similarly, the local temperature control in micro-process reactors has been identified as highly important to achieve efficient realization of various chemical reactions. Hence, understanding and modeling of heat transfer during evaporation process in microchannels are highly important for optimal design and thermal management of these applications. Despite the knowledge provided by many studies on flow and heat transfer characteristics in microchannels by high-speed videography and infrared thermography, development of novel simplified models for prediction of heat transfer mechanism inside a microchannel is still required. In this study, we model the heat transfer to a single nucleate vapor bubble which then expands to an elongated bubble during evaporation in the microchannel.

The model is a logical mix of empirical correlations and analytical models and is divided into two steps; (a) partially confined growth, the bubble expands from nucleation site until it fills the entire cross-section of the channel. (b) Fully confined growth, the bubble reaches the side walls,

begins to elongate axially in downstream direction. An initial bubble nucleus at the microchannel smooth wall with constant temperature is assumed. The initial condition is steady laminar flow with a constant inlet velocity. It is assumed that heat is transferred to the bubble only by evaporation of a thin liquid film. The heat flux through the contact area is equated to the uniform heat input to the wall q_w , implying that the thin liquid film at the wall has the negligible thermal capacity. The enthalpy of evaporation H_{lv} and the vapor density ρ_v are assumed constant. To estimate the heat transfer characteristics of vapor bubble growth during the evaporation inside of the microchannel, the time variation of liquid film thickness and the bubble nose position are evaluated. Finally, a time-averaged value of local heat transfer coefficient is obtained for a period of time using available heat transfer correlations for each heat transfer process separately. Results of the present model are compared to the results of a 3D simulations, where the bubble growth is modeled using the volume-of-fluids method with evaporation. Influence of the model assumptions is discussed based on the comparison of instantaneous and time-averaged results. Concluding, we assess the possibility of application of the presented model for an optimization of the micro heat-exchanger geometry and operational parameters.

The curvature of an evaporating meniscus in a pressure driven flow through cylindrical pores

Thomas Loimer (*TU Wien, Austria*)

08:50

The pressure driven flow of a vapor near saturation through anodic alumina membranes is considered. Anodic alumina membranes have very regularly spaced, cylindrical, straight pores with diameters between a few nanometers to some tens of nanometers. Due to the small pore size, there is a considerable pressure difference between the upstream and the downstream side of the membrane. The pressure is in a state close to saturation upstream of the membrane. Downstream of the membrane, the vapor is in a state far from saturation. However, due to the small pore size, there may be capillary condensation, and liquid flows through a part of the membrane. The liquid evaporates at a location within the membrane, in a field of a large pressure gradient in flow direction. The radius of curvature of the evaporating meniscus is calculated by applying the balances of mass, momentum and energy and observing the conditions at the interfaces. In addition, the real properties of the fluid are accurately described. Thus, for adiabatic flow, the Joule-Thomson effect is recovered. Due to the Joule-Thomson effect, a vapor close to saturation may condense due to the conduction of heat in downstream direction, not only due to capillary condensation.

Experimental data for the mass flow and the upstream and the downstream pressure is available, but the temperature field is not precisely known. The temperature field is calculated assuming either isothermal, adiabatic or diabatic flow. For adiabatic flow, there is no heat transfer from the downstream side of the membrane to the environment, while for diabatic flow, the downstream temperature of the membrane is the same as the upstream temperature. The radius of curvature of the meniscus within the cylindrical pores may be larger, or it may be smaller than the pore radius.

Depending on the assumptions regarding the temperature field, the computed radii of curvature of the menisci vary considerably. It can be concluded, that a precise knowledge of the temperature field is necessary, in order to determine the curvature of the evaporating meniscus. Models to deduce the temperature field from the temperatures at the upstream and the downstream surface of the membranes are presented.

The capillary rise as a benchmark for DNS wetting simulations

Dirk Gründing (*TU Darmstadt, Germany*)

Holger Marschall (*TU Darmstadt, Germany*)

Dieter Bothe (*TU Darmstadt, Germany*)

09:10

How does a liquid wet a surface and what is a suitable model to describe this phenomenon? These questions have been under investigation since the days of Newton and Laplace and are still an area of active research today.

A classical experiment to analyze the wetting phenomenon, is the rise of liquid between two planar plates. While a no slip condition on a wall boundary is a widely accepted approach to model fluid wall interaction, it yields diverging pressure and viscous dissipation towards the moving three phase contact line. For the solution of the full 2D problem, results are compared between an ALE interface tracking method, an algebraic interface capturing method (both OpenFOAM), as well as a geometric volume of fluid implementation, and a discontinuous Galerkin level-set front tracking approach. A comparison to the classical one-dimensional model solution for the rise of a liquid in a gap shows that the attempt to numerically solve the full 2D gap problem yields unusable results due to a strong mesh dependency.

To avoid the mesh dependency, a Navier slip boundary condition around the contact line is adopted. In addition, this approach reduces the severity of diverging fields towards the contact line. A typical physical slip length is of the order of a few nanometers as can be estimated from MD simulations. A price to pay for resolving the mesh dependency is that resolving such small length scales requires a significant mesh resolution around the contact line. In addition, the classical ODE describing the rise of liquid in a capillary does not include any slip on the capillary walls. A novel approximate model for capillary rise problem is presented that includes slip on the capillary walls. This also allows to use a slip length of the order of the capillary radius, hence significantly reducing the necessary mesh resolution for this test case. Comparing the results from solving the 2D problem and the novel model with slip length do not only show mesh convergent results, but also an excellent agreement in contrast to a comparison with the classical model.

ACKNOWLEDGEMENTS

We kindly acknowledge the financial support by the German Research Foundation (DFG) within the Collaborative Research Centre 1194 “Interaction between Transport and Wetting Processes”, Project B02“

The contact line advection problem

Mathis Fricke (*TU Darmstadt, Germany*)

09:30

Dieter Bothe (*TU Darmstadt, Germany*)

In a recent publication, we introduced the kinematic evolution equation for the dynamic contact angle. This equation expresses the fundamental relationship between the rate of change of the contact angle and the structure of the transporting velocity field. In this talk, we consider the geometrical problem of the passive transport of a hypersurface by a prescribed velocity field in the special case where the hypersurface intersects the domain boundary. This problem emerges from the discretization of continuum models for dynamic wetting. We employ the Volume-of-Fluid (VOF) method to solve the hyperbolic transport equation for the interface in both two and three spatial dimensions. The kinematic evolution equation leads to a system of ordinary differential equations serving as a reference to validate the VOF method. The geometrical reconstruction method for the interface is adapted at the domain boundary leading to an excellent agreement with the reference solution.

Numerical simulation of suction cavitation in hydrodynamic journal bearings

Marcus Schmidt (*HAWK Göttingen, Germany*)

09:50

Peter Reinke (*HAWK Göttingen, Germany*)

Tom Beckmann (*HAWK Göttingen, Germany*)

The prediction of cavitation in journal bearings is one of the current challenges in the field of computational fluid dynamics. Hydrodynamic journal bearings are used in a wide range of technical and industrial applications because they provide low friction and minimal wear. A failure of the bearing system during operation can be caused by suction cavitation. The cavitation of the fluid is known as a transfer process from of liquid phase to vapour phase of the fluid by lowering the pressure at an approximately constant temperature under a critical vapour pressure. The implosion of vapour cavities adjacent to the surface of the bearing liner stresses the liner material which in turn can lead to material erosion. The particular case of suction cavitation can be observed, if the bearing is operated under high loads resulting in high eccentricity between shaft and bushing combined with a significant increase in gap width. Suchlike operating conditions are not uncommon for internal combustion engines with a power of 0.1 to 1.0 MW per cylinder. As a result of the transient shaft displacement a suction effect builds up within in the lubricating film accompanied with a strong pressure gradient. Due to the fluid dynamics of the lubricant film flow at the given pressure gradient, the liquid can only equalize the void caused by the shaft displacement until the fluid pressure reaches the vapor pressure and then vapor is generated. The vapor forms a three-dimensional layer across the lubrication gap. Whereas, current flow calculations for hydrodynamic journal bearings are carried out by means of 2D methods which are limited to analyze the three-dimensional and transient flow in those areas of the journal bearing where cavitation occurs. This work presents the application of a transient, 3D numerical simulation of the two-phase fluid flow in a journal bearing under conditions of cavitation. The numerical simulations were performed using the code OpenFOAM, which is based on the finite volume method and uses time-dependant three-dimensional, incompressible Navier-Stokes equations. The study on hand discusses the influence of minimal gap width and displacement velocity vs. the structure of the vapour distribution. The numerical results include images of complex three-dimensional flow structures and vapor distributions inside the lubrication gap.

Choking and hydraulic jumps in laminar flow

Bernhard Scheichl (*Technische Universität Wien, Austria*)

10:10

Robert I. Bowles (*University College London, UK*)

Georgios Pasiadis (*University College London, UK*)

The (steady) viscous hydraulic jump still represents research in progress rather than a finalised edifice. The rigorous approaches of the last decades showed how this phenomenon is intrinsically associated with a bifurcation of the upstream flow adjacent to the guiding rigid plate, aligned perpendicularly to the direction of gravity. This initiates a process of viscous-inviscid interaction and reflects the likewise essential upstream influence, originating in suitable downstream conditions that trigger the transition from super- to subcritical flow (these notations have a well-defined meaning). However, the challenge of a self-consistent formulation involving the latter mechanism has only been mastered conclusively for relatively weak jumps, connecting states slightly detuned from choking conditions over a correspondingly short streamwise length in boundary-layer flows. The smooth jump in developed flow, however, is terminated by locally choked flow, as predicted by a marching singularity in the solution to the underlying shallow-water problem. Its localisation is associated with the trailing edge of the plate, but how this flow at critical conditions passes the latter and is finally transformed into a downfall is a topic under consideration yet.

We present recent advances in the establishment of a closed asymptotic theory for a developed jump. Currently, the global Froude number expressed in terms of the slenderness parameter of the flow is taken as so large that deviations from the parabolic shallow-water limit are predominantly due to streamline curvature. Then the flow only "chokes weakly", i.e. in its near-plate portion. A novel canonical interaction problem provides the regularisation of the accordingly weak form

of the trailing-edge singularity on a streamwise length scale much smaller than the global one describing the full jump and a context to the aforementioned transcritical boundary-layer flow. As a side aspect, this scenario completes a long-standing debate on an analogous singularity and its smoothing occurring in interactive hypersonic boundary layers. We then demonstrate how that interactive flow regime gives way to a further one encompassing the edge on a reduced scale and accounting for the downfall process.

This analysis captures the upstream influence and how it controls the bifurcation process in a correct manner. Furthermore, it paves the way for a complete rational description of the hydraulic jump for moderately large Froude numbers on a global length scale, measuring the distance from the virtual origin of the supercritical flow to the plate edge. Differences to the axisymmetric jump over a spinning disc are addressed in brief.

S11.07 | Interfacial flows

Date: February 21, 2019
Room: HS 02

14:00-16:00

Numerical and experimental investigation on the flow behavior of liquids in narrow gaps

Luca Luberto (*TU Kaiserslautern, Germany*)
Kristin de Payrebrune (*TU Kaiserslautern, Germany*)

14:00

Lapping is a manufacturing processes with geometrically undefined cutting edges and is used to produce technical surfaces with high dimensional and shape accuracy.

To predict the manufactured surface, a process model will be developed, which combines models of the material removal mechanism, the kinematic of lapping particles, and the flow of the lapping liquid. Due to the incoherent structure of the lapping liquid (loose lapping grains within the liquid) this can only be done by a multiphysical model.

In a first step, only the flow behavior of the liquid without lapping particles is examined numerically and experimentally. Therefore, particle image velocimetry is used to measure the flow within a gap with a fixed bottom plate and a translatory moving upper plate. The gap between both plates and the velocity of the upper plate can be varied. The experimental setup is rebuild as a CFD model. Also in the numerical study, the velocity of the upper plate and the gap is varied and the results are critically compared with experiments.

The CFD model helps to analyze further parameters, as the influence of the velocity on the flow. Finally the model will be used to analyze the interaction between lapping particles and lapping liquid, which is very important to study the material removal mechanisms in lapping.

Convective dissolution in porous media: experimental investigation in Hele-Shaw cell

Marco De Paoli (*TU Wien, Austria*)
Mobin Alipour (*TU Wien, Austria, University of Udine, Italy*)
Alfredo Soldati (*TU Wien, Austria, University of Udine, Italy*)

14:20

Global consumption of fossil fuels, responsible for greenhouse effect, has doubled over the last decades, with no sign of drop. A possible solution to reduce the amount of carbon dioxide (CO₂) in the atmosphere has been identified with the CO₂ sequestration strategy. In this process, liquefied CO₂ is stored in saline aquifers, geological formations characterized by large values of the permeability. Accurate measurements and modeling of dissolution processes play a key role in understanding the long-term behavior of liquid CO₂ injected in these underground geological

formations. Currently, experiments can easily reach Rayleigh numbers not achievable with the numerical simulations. In this work, we aim at performing experimental measurements from a Hele-Shaw to prove that convective fingers have a huge impact on the dissolution dynamics. We analyze the experimental results obtained at large Rayleigh numbers (i.e. when convection dominates over diffusion), currently still unachievable via numerical simulation, and we explore the implications of these results on the CO₂ convective dissolution in saline aquifers.

Effective permeability of a flow through a packed bed of beads between two walls affected by overlapping wall effects

Konrad Boettcher (*TU Dortmund, Germany*)

14:40

Tim Neumann (*TU Dortmund, Germany*)

Peter Ehrhard (*TU Dortmund, Germany*)

In a packed bed of beads the spheres usually are distributed randomly. But the walls confining the packed bed disturb the randomness and characteristically arrange the spheres. Therefore, the porosity gets a function of the wall distance, which is examined well in literature for packed beds in cylinders. In this so-called wall effect, the porosity has the form of a damped oscillation. Here, we investigate the porosity profile of a packed bed of monodisperse spheres in a rectangular container and the effect onto the porosity profile if the distance of the opposing walls is reduced, so that the wall-effect regions start to overlap. The profiles are experimentally determined by using a displacement method, which is modified to avoid corrugated interfaces.

In further experiments, a resin is poured into packed beds and sectional views parallel to the wall are cut after curing. The mean pore diameter is then determined, showing that the corresponding constant value of the Ergun equation does not fit that good in the wall effect region. Therefore, the characteristic length scale in the Ergun equation is modified by using a non-constant mean pore diameter determined by Cai and Yu (2010) using a fractal method. The velocity profiles are computed numerically and are compared with experimental results. In the experiments, particle image velocimetry is engaged in an optically-matched bed of glass spheres.

Effective permeabilities considering the wall effect and wall friction are determined numerically for different wall distances and bulk porosities. Using these results the simple Darcy law can be used for calculating pressure drops of flows through thin rectangular geometries considering the wall-effect and friction.

Numerical investigation of aerosol deposition on single fibers

Saravanan Mohan (*TU Dortmund, Germany*)

15:00

Jayotpaul Chaudhuri (*TU Dortmund, Germany*)

Lutz Gödeke (*TU Dortmund, Germany*)

Peter Ehrhard (*TU Dortmund, Germany*)

The aerosol filtration technique requires extensive studies, due to its wide applications found in health, environment and industry. The simulation of aerosol filtration over fibrous filters involves the numerical investigation of motion and capture of particles (aerosols) under different fluid operating conditions.

The capture of aerosol in fibrous filters involves the following deposition mechanisms: Impaction, interception, diffusion and gravitation. The motion of the particles is governed by the relevant forces acting on the particles. Due to the dilute concentration of the aerosol, the motion due to particle interaction can be neglected. The particles are removed by a fibrous filter when they collide and attach to the surface of the fiber. An Euler-Lagrangian approach is engaged to simulate the particle trajectory. The air flow field (continuum phase) is simulated in Ansys[®]CFX (Euler) and the particle trajectories (dispersed phase) are computed by Lagrangian simulations

in MATLAB. Since the dispersed phase movement is predicted based on constant continuum flow field, a one-way coupling approach is present.

The fibrous filters consist of a large number of fibers of uniform size and random orientation and position. We consider a single fiber placed normal to the airflow and analyze several deposition mechanisms.

The efficiency at which the particles are collected by a single fiber from an aerosol stream is called single-fiber efficiency E_{Σ} , which is highly dependent on particle size. The particle motion is also affected by a diffusion mechanism, where the dispersion of particles due to Brownian motion follows a Gaussian distribution. The diffusion coefficient can be inferred from the mean distance travelled by the particle and agrees well with the theoretical diffusion coefficient calculated from the Stokes-Einstein equation. The influence of the diffusion mechanism becomes significant at particle sizes below $0.2\mu\text{m}$.

The single-fiber efficiency is determined considering all deposition mechanisms. The extension of the single-fiber to 3D-models and real fibrous filter structure models with random fibers arrangements is in development.

Flow through randomly-oriented fibrous filters

Jayotpaul Chaudhuri (*TU Dortmund, Germany*)

15:20

Konrad Boettcher (*TU Dortmund, Germany*)

Peter Ehrhard (*TU Dortmund, Germany*)

Fibrous filters are often employed to remove dispersed aerosol particles from a gas stream due to low cost, high capture efficiency and low pressure drop. This kind of filtration is a depth-filtration process which is widely used in process industries to remove particulate matter from exhaust gases, or in compressed air applications to filter oil particles introduced during the compression process. The performance of such a filter medium is judged based on its capture efficiency and its pressure drop characteristics. Estimating these parameters without setting up experimental investigations of each filter medium is beneficial for choosing and developing optimal filters.

In the present study, numerical simulations using ANSYS CFX are used to predict the pressure drop caused due to an air flow through a randomly oriented fibrous filter medium. A fictitious domain approach is used to simulate solid fibers without the need to create a case-specific mesh for different fiber alignment. This method is used to model several fibers in 3D with various degrees of freedom in orientation within a defined domain size. The domain size is varied till the average solidity of the medium converges to the desired filter solidity. Furthermore, images from scanning electron microscope (SEM) of actual filter material are investigated to establish restrictions in the fiber orientation. With the optimal representative domain size and fiber orientation restriction, several simulations with varying Reynolds number, solidity and orientation are carried out, and the pressure drop across the filter is inferred.

The pressure drop data are used to develop a correlation which can be used by industry or in further research to approximate the pressure drop through a fibrous filter. It is found that the computed pressure loss through randomly oriented fibers is significantly lower than pressure loss through ordered fibers. This can be explained by the formation of channels with low resistivity within the filter medium, where the bulk of the fluid flows, resulting in a lower overall pressure drop.

Estimating the efficiency of flow-through filters for marine diesel engine applications using a CFD-QMOM approach

Axel Fiedler (*MAN Energy Solutions SE, Augsburg, Germany*)

15:40

Manuel Kleinhenz (*MAN Energy Solutions SE, Augsburg, Germany*)

Andreas Döring (*MAN Energy Solutions SE, Augsburg, Germany*)

The reduction of particulate emissions from diesel engines is a major challenge for engine manufacturers. While a majority of applications can be equipped with wall-flow filters to meet emission limits, this approach has little prospect of success for most marine large-bore diesel engine applications. The use of fuels with high ash content leads to clogging of the filter and makes the operation costly and maintenance-intensive. Flow-through filter technologies can be an advantageous alternative for these applications as they feature beneficial back-pressure and clogging behavior while still reducing the particulate matter of the exhaust [1]. These filters work by forcing the particle-laden flow through small, sinuous channels and collect the solid fraction at the walls. In the case of diesel exhaust, the soot particles are then converted to gaseous carbon dioxide using the NO₂ content of the exhaust gas.

Numerical methods are used widespread across a variety of industries to reduce the development time and cost of new products. In the case of flow-through filters, numerical methods could be used to find an optimal geometry with respect to back-pressure and filtration efficiency. Unfortunately the transport and interaction of diesel soot particles include effects on a small time and length scale such as Brownian motion. These effects lead to high computational costs if Lagrangian particle tracking is applied [2].

Therefore, the use of other approaches like the quadrature method of moments (QMOM) is of interest. This approach uses a set of passive scalars (moments) which are transported according to the flow field to represent the particle size distribution [3]. Source terms in the transport equations of the moments account for aggregation and deposition of the particles [4]. In the presented work a QMOM approach is developed and implemented in a commercial CFD code to estimate the filtration efficiencies of different flow-through filter geometries. The results are validated using measurements from model soot as well as real engine experiments.

[1] Heikkilä et al., *Journal of the Air & Waste Management Association* 59, 1148-1154 (2009)

[2] Bensaïd et al., *Chemical Engineering Journal* 154, 211-218 (2009)

[3] Marchisio et al., *AIChE Journal* 49, 1266-1276 (2003)

[4] Guichard et al., *Journal of Aerosol Science* 104, 16-31 (2017)

S11.08 | Interfacial flows

Date: February 22, 2019

08:30-10:30

Room: HS 02

Modeling and simulation of the desalination process using CO₂ hydrate

Jawon Ha (*LSTME Busan, Republic of South Korea*)

08:30

Cornelia Rauh (*TU Berlin, Germany*)

Antonio Delgado (*FAU Erlangen-Nuremberg, Germany*)

Seawater can be converted into fresh and potable water by desalination, a process where salts are removed from the seawater. Hydrate desalination is considered to be a promising alternative for the desalination process compared to traditional methods and it is a multiphase fluid flow process where gas hydrates form. These are non-stoichiometric crystalline compounds that are formed by gas and water molecules at specific conditions of temperature and pressure.

Hydrate desalination is in principle more economical compared to other processes since salt is separated from water during the hydrate formation. Therefore, this process is expected to be more energy efficient compared to thermal evaporation or nanofiltration, since both processes require additional energy for separating the salts from water.

In this work, we simulated the whole desalination process by means of High-level Petri net, the so-called reference nets. They provide high flexibility with respect to the dynamic of the process and the required implementation of different modeling and simulation approaches. In addition, we constructed a SQL database with the initial values of pressure, temperature and

salt concentration of each device. Moreover, we also specify the reaction involved and created a graphical user interface (GUI) to visualize the flow balance of each device. After simulating the whole process, the results of the flow balance are stored in the SQL database. These results are visualized as plots of energy and mass against time in the GUI. The actual values of the energy and mass are used to calculate the energy consumption of each device and of the whole process as well.

Proceedings in fluidesign

Tom Beckmann (*University of applied sciences HAWK Goettingen, Germany*) 08:50
Peter Reinke (*University of applied sciences HAWK Goettingen, Germany*)
Marcus Schmidt (*University of applied sciences HAWK Goettingen, Germany*)

This work presents the process of designing a cavitating fluid for the lubricant flow in journal bearings. Hydrodynamic journal bearings are used in a wide range of technical and industrial applications because they provide low friction and minimal wear. The principal operational feature of these bearings is an eccentrically rotating shaft inside the bushing resulting in convergent and divergent lubrication gaps of just a few micrometers in size between the shaft and the bushing. For the particular case of internal combustion engines the displacement of the shaft is transient with strong variations in eccentricity and displacement velocity. Hence, the flow inside the lubrication gap is transient and three-dimensional. Investigations of the flow inside journal bearings are technically challenging. The following geometrical and physical conditions have to be tackled: small fluid-gap dimensions, optical accessibility, Reynolds and cavitation similarity. The combination of these conditions requires a scaled journal bearing experiment with a special fluid that fulfils the cavitation condition. The most important component of the experimental setup is the fluid in order to create the desired flow conditions. The authors of this work have proven that a cavitating fluid can be designed to specification by applying the new approach to the cavitating Taylor-Couette flow. The proper fluid design has to fulfill three criteria: physical compatibility, Reynolds analogy and cavitation number at the operating point. Physical compatibility stems from material specifications of the apparatus and the need to provide optical accessibility by providing identical refractive indices of fluid and housing. The fluid must be chemically compatible with acrylic glass of the apparatus preventing unwanted reactions. Laser-optical measurements are the most suitable means to obtain significant data of the flow field inside the lubrication gap. The relation of dynamic pressure at the operating point and mechanical dimensions of the apparatus defines the viscosity necessary to fulfil the Reynolds analogy. Finally, the cavitation number in relation to the combination of dynamic and static pressure provides the target vapor pressure of the special fluid. Thus, the present work describes the development of a special fluid applicable for journal bearings in model scale, which not only fulfills pressure and cavitation analogy but also features a favorable refractive index and a chemical suitability for the task. Furthermore, the work shows results of a cavitating flow in a small gap arrangement by means of the designed fluid.

A CFD model for simulating the electron beam welding of a CrMnNi-steel

Sebastian Borrman (*TU Bergakademie Freiberg, Germany*) 09:10
Rüdiger Schwarze (*TU Bergakademie Freiberg, Germany*)

For the application of new materials, such as CrMnNi TRIP/TWIP-steels, a detailed understanding of fabrication processes, like electron beam welding (EBW), is needed. In this regard, numerical models are getting more and more attention as an addition to experimental investigations.

A CFD model for needs to contain many occurring effects, such as phase change phenomena (melting, solidification, boiling together with latent heat release and consumption), thermocapillary convection, recoil pressure, heat conduction and the energy input by the electron beam. This is accompanied by fluid flow in the melt pool and formation of the melt and welding seam geometry. Furthermore, a detailed knowledge about the temperature sensitive thermophysical properties is required. Due to the partially melting behavior of the steel alloy, a mushy zone evolves during melting and solidification and needs to be considered as well. The interplay of all this effects leads to a complex multiphysical problem.

The presented transient 3D model was implemented into OpenFOAM in order to provide an extendable fundament for welding simulations. It consists of a combined heat source with a double ellipsoid for the upper nail head part of the fusion zone and a conical part for the lower, narrowing region. The influence of temperature dependent properties has been found to be very significant, especially for the welding seam formation. The complexity of heat source as well as the number of free parameters can be reduced, if accurate properties are used.

A comparison of the simulated welding seam with a weld that has been produced in an electron beam chamber shows very good agreement. A parameter study shows a strong dependence of the weld pool and seam formation on the steel properties. The formation of the typical tear drop form of the weld pool is also achieve, when temperature sensitive properties are used. Further refinements and implementations of physical effects can now be tackled in order to exactly reflect the fluid flow in the weld pool.

S12 | Waves and acoustics

Organiser: Manfred Kaltenbacher (*Technische Universität Wien, Austria*)
Barbara Kaltenbacher (*Alpen-Adria Universität Klagenfurt, Austria*)

S12.01 | Waves and acoustics

Date: February 19, 2019
Room: HS 34

08:30-10:30

Evaluation of source signature during Full Waveform Inversion for seismic reconnaissance in tunneling

Christopher Riedel (*Ruhr-University Bochum, Germany*) 08:30
Khayal Musayev (*Ruhr-University Bochum, Germany*)
Matthias Baitsch (*Bochum University of Applied Sciences, Germany*)
Klaus Hackl (*Ruhr-University Bochum, Germany*)

By transmitting seismic waves in the ground the spread, reflected and refracted waves can be recorded at different positions. The arising seismograms contain information of the geology, which can be evaluated with the Full Waveform Inversion (FWI).

For the application of FWI for reconnaissance in tunneling extensive information has to be provided to achieve an appropriate model of the geology in front of the tunnel face. Such information are the position and geometry of reflecting boundaries, exact position of sources and receivers, a proper initial model of the distribution of the material parameters. The signal, which is transmitted by the senders, has also an influence on the inversion. Even if the intended source function is known, the effective signal depends on the transfer functions between sender-soil and soil-receiver and its identification is challenging.

To avoid cumbersome investigations on the source function in advance we applied a simultaneous identification of the source signature during the FWI in the frequency domain. For synthetic models of a 2D tunnel configuration with disturbances, we will show how the calculated source signature of a frequency converges to the real source signature during the iterations of the FWI. The influence of different sender and receiver configurations will be analyzed. Furthermore, the influence of the simultaneous evaluation of the source signature on the results of the FWI will be evaluated. In a post-processing step of the FWI, the source signature of the whole frequency spectrum will be determined.

Initial source estimation of the wave equation with applications to photoacoustic tomography

Alexander Beigl (*University of Vienna, Austria*) 08:50
Jarle Sogn (*Johannes Kepler University, Austria*)
Otmar Scherzer (*University of Vienna, Austria*)
Walter Zulehner (*Johannes Kepler University, Austria*)

Photoacoustic Tomography (PAT) is a hybrid imaging modality which combines the benefits of high contrast from electromagnetic absorption and high resolution via ultrasonic waves. A specimen of interest is illuminated by a short laser pulse. The absorbed electromagnetic energy creates a heating of the probe which induces an acoustic pressure wave caused by rapid thermal expansion. The spatially varying initiated pressure wave is assumed to be proportional to the

electromagnetic absorption which shows high contrast between various kinds of tissues. Hence the initial source reconstruction of the acoustic pressure field constitutes a promising diagnostic tool.

Mathematically, the propagating pressure wave is modeled with the homogeneous acoustic wave equation on the whole unbounded spatial domain. The inverse problem in PAT is to reconstruct the initial pressure distribution given time-dependent measurements of the pressure wave at the boundary of a bounded domain which contains the support of the initial pressure distribution. The inverse PAT problem motivates our research. In our work we address the estimation of the inverse source for the acoustic equation on a bounded domain and consider time-dependent measurements of the wave on the boundary of a compactly contained subset of the original computational domain. Given (noisy) data, we aim at minimizing the data discrepancy plus a penalization term and introduce Lagrangian multipliers to complement the constraint of the wave equation. We discuss well-posedness of the corresponding saddle point problem and conclude the theory with numerical experiments. Finally, we discuss to which extent the theory applies for the original PAT problem on the unbounded domain.

Numerical method to determine the inverse solution of two impacting rods of non-constant cross section

Jens Burgert (*KIT Karlsruhe, Germany*)

09:10

Wolfgang Seemann (*KIT Karlsruhe, Germany*)

Impacting rods are used in several scientific experiments and in everyday tools such as drilling machines. For deep hole drillings, the efficiency of the drilling process can be improved by shaping the longitudinal wave that is transmitted through the drill rod to the drill bit [1]. The approach implemented in this contribution is to adjust the longitudinal wave shape by varying the geometry of the impacting piston.

In general, numerical methods have to be applied to determine the wave propagation of two impacting rods since analytical solutions only exist for certain cross sections [2]. Furthermore, the collision leads to a sudden jump of the velocity and therefore to a non-smooth contact problem which is computationally expensive to calculate.

In this contribution, an approach to calculate the inverse solution of impacting rods of non-constant cross section is presented. The idea is to approximate the geometries of the rods by piecewise constant cross section segments. The solution of the wave propagation on these segments is well known by the d'Alembert solution. At the cross section changes, transition conditions have to be formulated which can be derived by claiming force- and displacement equilibrium. The inverse solution is calculated iteratively, which means that the rod geometry of the first rod is determined for a prescribed stress over time at one position of the second rod. The main advantage of the iterative approach over an optimization is the considerable shorter calculation time. Moreover, the iterative approach results are very accurate.

[1] Lundberg, B. and Collet, P., Optimal wave with respect to efficiency in percussive drilling with

integral steel, *International Journal of Impact Engineering*, 37, page 901- 906 (2010).

[2] Guo, S. and Yang, S., Wave motions in non-uniform one-dimensional waveguides, *Journal of Vibration and Control*, 18(1), page 92-100 (2011).

Frequency-bounded delay and sum: a modified damage detection method in thin walled plates

Afshin Sattarifar (*Ruhr University Bochum, Germany*)

09:30

Tamara Nestorović (*Ruhr University Bochum, Germany*)

Structural Health Monitoring (SHM) has established itself as a powerful tool to observe the reliability of structures. In addition, SHM systems enable the early prediction of the presence of the material damage in a structure. There are generally two families of the SHM methods, ultrasonic guided wave-based, and vibration-based SHM. This study is concerned with the former methodology. Lamb waves, as ultrasonic guided waves, have shown a great capability of identifying and localizing damage in metallic and composite structures. Excitation, as well as measurement of Lamb waves, in structures is possible via implementing piezoelectric transducers. Due to durability, low power consumption, and light weight of piezoelectric transducers, the feasibility of guided wave-based methods are enhanced.

The delay-and-sum methodology is implemented in the current study to depict the probability of the presence of the damage on an Aluminum plate. Contrary to previous researches, in this work, a systematic procedure for choosing the frequency of excitation and the type of excitation signal is considered. Additionally, by introducing a modified version of the algorithm, the most appropriate frequency ranges for several setups of plates and damage locations are provided. This modification serves to obtain a more accurate location of the damage as well as to reduce the presence of the artifacts. Firstly, the propagation of the Lamb waves in the plate is modeled numerically by means of the commercial finite element package, ABAQUS. Furthermore, the effect of choosing different solver setups on the accuracy of the numerical simulation is regarded. Secondly, to show the practicality of the method, a comparable experimental setup to that of the numerical simulation is made, in which piezo patches are utilized to excite the Lamb wave and to measure the corresponding displacement on the plate as well. Analysis of the experimental results shows the viability of the method to identify the introduced damage on the structure.

Sensor positioning in the context of wave-based damage identification in dams

Ina Reichert (*Bauhaus-Universität Weimar, Germany*)

09:50

Muyiwa Alalade (*Bauhaus-Universität Weimar, Germany*)

Tom Lahmer (*Bauhaus-Universität Weimar, Germany*)

Dams and their adjoining reservoirs play an important role in the drinking water supply as well as in the flood defense. Their world-wide use and possible massive devastation due to dam failures make the monitoring of the structural health of these huge structures imperative. Therefore, it is necessary to identify faults/damages in the dams' structure non-invasively in order to proceed with the current use. Additionally, monitoring of these huge structures is very complex, time-consuming and costly. To circumvent the aforementioned challenges, an inverse analysis, here an enhanced, regularized, cyclic full-waveform inversion is proposed based on wavelengths between seismic and ultrasonic waves.

Parameters of the dam material, such as stiffness, density and permeability, are estimated in synthetic experiments.

Having this, an optimal design of experiment approach is used to obtain an optimal number of sensors and also to identify the most informative positions regarding the reconstruction quality. An optimized sensor layout may further improve the efficiency of the solution of the inverse problem.

Simulation of vibrational sources and vibroacoustic transfer in wind turbine drivetrains

Frank Ihlenburg (*Hamburg University of Applied Sciences, Germany*)

10:10

Thomas Grätsch (*Hamburg University of Applied Sciences, Germany*)

Marc Zarnekow (*Hamburg University of Applied Sciences, Germany*)

With the increasing usage of renewable energy suppliers like wind or biogas, electricity is nowadays produced in many distributed locations that are often situated within or close to

inhabited areas. Over the last years, the control of noise emission from wind turbines has become an issue of growing attention and strict regulation. Of particular importance are tonalities in the noise spectrum. These tonalities in the far-field spectrum can be traced back to mechanical sources within the drivetrain like the gear box and the generator. The focus of our research is on the simulation of transfer paths from the vibrational sources to the radiating components, with the goal of identifying efficient design measures for the reduction of tonal noise. We show how hybrid analytical-numerical models can link experimental results from far-field measurements to the gear transmission error. Particular attention is then given to the precise modeling of structural sound propagation through the drivetrain. As the frequency range of engineering interest is broad, a fine local resolution of the discrete models is required. Various methods of model order reduction are used to facilitate an efficient evaluation of engineering design variants. References:

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S12.02 | Waves and acoustics

Date: February 19, 2019
 Room: HS 34

16:30-18:30

Adaptive discontinuous Galerkin methods for the Helmholtz equation

Scott Congreve (*University of Vienna, Austria*)

16:30

Joscha Gedicke (*University of Vienna, Austria*)

Ilaria Perugia (*University of Vienna, Austria*)

An hp adaptive refinement procedure for discontinuous Galerkin (DG) discretizations of the Helmholtz equation will be presented.

The Helmholtz equation with impedance boundary condition in two space dimensions will be taken as a model problem, and polynomial-based DG approximations with stabilization terms containing jumps of the traces, as well as jumps of the normal components of the gradients at the interelement boundaries, will be considered. These methods are unconditionally well-posed, and are therefore well-suited also when the adaptive procedure is started in the pre-asymptotic regime.

The a posteriori error analysis we will present is based on a local reconstruction of equilibrated fluxes applied to an auxiliary shifted Poisson problem with inhomogeneous Neumann boundary conditions. With respect to the standard framework of equilibrated fluxes for elliptic problems, additional terms related to the DG treatment of inhomogeneous impedance boundary conditions appear in the estimator, together with an extra lifting operator, which is required in the definition of the discrete gradient. The presence of this term is due to the additional gradient stabilization terms in the DG discretisation of the Helmholtz problem. The error due to the nonconformity of the approximation spaces is controlled by a potential reconstruction.

The considered a posteriori error estimator is proven to be both reliable and efficient, outside the regime of pollution, up to generic constants which are independent of the wave number, the polynomial degrees, and the element sizes. By construction, the estimator captures possible singularities of the solution correctly. In contrast to residual based a posteriori error estimators,

the presented error estimator is robust in the polynomial degree. Some numerical experiments will be presented, in order to confirm the efficiency of hp-adaptive refinement strategies based on the presented a posteriori error estimator.

Covariant and contravariant complex stretching for time dependent wave propagation problem solved with discontinuous finite elements

Bernard Kapidani (*Technische Universität Wien, Austria*)

17:10

Joachim Schöberl (*Technische Universität Wien, Austria*)

Scalar and vector hyperbolic systems of PDEs lead to wave solutions in acoustic and electromagnetic problems. The effort of finding accurate and efficient numerical approximations to this problem in the framework of the Finite Element Method (FEM) has led to the recent huge development of Discontinuous Galerkin Finite Elements which, by partially or completely neglecting the continuity constraints on test and trial functions, allow an explicit integration in time of the equations. This contribution deals with the coupled first order formulation of the governing equations and the subsequent efficient implementation in the FEM library NGSOLVE of the method by means of orthogonal polynomials and exploitation of the appropriate covariant/contravariant Piola mapping of the fields from master to physical finite elements, the choice of which is intimately connected to the nature of the physical problem.

Furthermore, the natural setting for such propagation problems in the time dependent case is usually an unbounded physical domain. To accommodate for these in the discrete formulation, non reflecting boundary conditions are needed. Artificial material layers which provide reflectionless absorption of waves via complex transformation are the most practically proven solution in this respect. In dealing with this, the present contribution shows that the mappings introduced play a fundamental role in the understanding and correct systematic discretization of such absorbing layers on a finite element mesh for the acoustic wave equation, and the time dependent Maxwell equations.

An explicit Mapped Tent Pitching scheme for wave equations

Jay Gopalakrishnan (*Portland State University, USA*)

17:30

Joachim Schöberl (*TU Wien, Austria*)

Christoph Wintersteiger (*TU Wien, Austria*)

We present a new numerical method for solving the wave equation, which is also suitable for general linear hyperbolic equations. It is based on a unstructured partitioning of the spacetime domain into tent-shaped regions that respect causality. Provided that an approximate solution is available at the tent bottom, the equation can be locally evolved up to the top of the tent. By mapping tents to a domain which is a tensor product of a spatial domain with a time interval, it is possible to construct a fully explicit scheme that advances the solution through unstructured meshes. Due to the special structure of the mapped equation, standard Runge Kutta schemes lead to a convergence order reduction. To overcome this issue we introduce the structure-aware Taylor time-stepping (SAT) technique. These fully explicit Mapped Tent Pitching (MTP) methods allow variable time steps and local refinements without compromising high order accuracy in space and time. The resulting algorithms of these MTP methods are highly parallel and utilize modern computer architectures extremely well.

New mass-lumped tetrahedral elements for 3D wave propagation modelling

Sjoerd Geevers (*University of Vienna, Austria*)

17:50

W.A. Mulder (*Shell Global Solutions International BV & Delft University of Technology, the Netherlands*)

J.J.W. van der Vegt (*University of Twente, the Netherlands*)

We present a new accuracy condition for constructing mass-lumped finite elements. This new condition is less restrictive than the one that has been used for several decades and enabled us to construct new mass-lumped tetrahedral elements of degrees 2,3, and 4. The new degree-2 and degree-3 elements require 14 and 32 nodes, respectively, while the degree-2 and degree-3 elements currently available in the literature require 23 and 50 nodes, respectively. Mass-lumped tetrahedral elements of degree 4 had not been found until now.

The resulting mass-lumped finite element method is suitable for 3D wave propagation problems, since it can accurately capture the effects of a complex geometry and since it results in a fully explicit time-stepping scheme. A dispersion analysis and several numerical tests illustrates the efficiency of this new method. In particular, they illustrate a significant reduction in degrees of freedom, number of time steps, and computation time for a given accuracy compared to other finite element methods, such as the previous mass-lumped finite element methods or the discontinuous Galerkin method.

L-sweeps: a scalable parallel high-frequency Helmholtz solver

Matthias Taus (*Massachusetts Institute of Technology, USA*)

18:10

Leonardo Zepeda Núñez (*Lawrence Berkeley National Laboratory, USA*)

Russell J. Hewett (*Virginia Tech, USA*)

Laurent Demanet (*Massachusetts Institute of Technology, USA*)

In many science and engineering applications, solving time-harmonic high-frequency wave propagation problems quickly and accurately is of paramount importance. In this talk we concentrate on fast solution techniques. It is historically challenging to obtain fast solution strategies for high-frequency problems.

Recently, there have been many advances in the development of fast solvers for such problems, including methods which have linear complexity with respect to the number of degrees of freedom. While most methods scale optimally only in the context of low-order discretizations and smooth wave speed distributions, the method of polarized traces has been shown to retain optimal scaling for high-order discretizations, such as hybridizable discontinuous Galerkin methods and for highly heterogeneous (and even discontinuous) wave speeds. However, to date, this method relies on a layered domain decomposition together with a preconditioner applied in a sweeping fashion, which has limited straight-forward parallelization.

In this work, we introduce L-sweeps, a new fast solution strategy that, similar to the method of polarized traces, can be applied to essentially any discretization but, in addition, reveals more parallel structure than any previously proposed strategy. In particular, for a single right-hand side our method scales as $O(n)$ in a distributed parallel environment where $n = N^{1/d}$, N is the number of degrees of freedom, and d is the problem dimension. Similar to the method of polarized traces, additional speed can be gained by pipe-lining several right-hand sides.

We motivate and introduce the method and present numerical examples to corroborate our claims.

S12.03 | Waves and acoustics

Date: February 20, 2019

08:30-09:30

Room: HS 34

Towards space-time boundary element methods for retarded potential integral equations

Dominik Pözl (*Graz University of Technology, Austria*)

08:30

Martin Schanz (*Graz University of Technology, Austria*)

Many acoustic and electromagnetic scattering problems are posed on unbounded domains with bounded boundary. Boundary element methods are an elegant tool for such problems, since they require a discretization of the boundary only. In this talk, we discuss the development of a space-time boundary element method for the wave equation in 3d. While most existing approximation methods discretize space and time separately, we establish a discretization scheme that does not rely on this separation. The key idea of such space-time methods is to treat the time variable as if it were an additional spatial coordinate. This enables the application of well-established finite and boundary element technology for stationary problems to time-dependent problems.

The discretization is based on a decomposition of the lateral boundary of the space-time cylinder into an unstructured tetrahedral mesh. On this mesh, standard finite element spaces, i.e. spaces of piecewise polynomial functions, are used to approximate the surface densities. A pivotal challenge within space-time boundary element methods is the accurate and robust computation of the boundary integral operators. In the case of the 3d wave equation they integrate along the intersection of the boundary of the backward light cone and the lateral boundary of the space-time cylinder. Due to this special structure these operators are also known as retarded potentials. Since these integrals can be quite complicated we restrict our considerations to collocation methods only. For tetrahedral space-time meshes we provide an accurate and robust numerical integration scheme for the pointwise evaluation of retarded layer potentials. The talk concludes by discussing numerical examples that illustrate the capacity of the method.

Generalization of adaptive cross approximation for time-domain boundary element methods

Anita Maria Haider (*Graz University of Technology, Austria*)

08:50

Martin Schanz (*Graz University of Technology, Austria*)

The investigation of wave propagation in elastic media is of great significance for a variety of engineering applications. An approximate solution of the corresponding initial boundary value problem is achieved by means of the boundary element method. The underlying boundary integral equations are of convolution type in time, which can be approximated by the convolution quadrature method (CQM). In addition, a generalization of the convolution quadrature method overcomes the restriction to solve time dependent problems only with constant time step size. However, the generalized CQM requires excessive amounts of memory. To get rid of this issue we carry out a low rank approximation using the adaptive cross approximation (ACA). This method has already been successfully applied to scalar-valued problems such as the scalar wave equation. Promising results have already been achieved for the extension of the ACA to vector-valued unknowns, for instance for elastodynamics in the frequency domain. The extension of the ACA to approximate a three-dimensional array of data is proposed in this talk. In particular, we perform an approximation on a set of boundary element matrices in the Laplace domain that occur by solving problems like elastodynamics based on the convolution quadrature boundary element formulation. The reduction of memory requirements and computation time while retaining a good quality of the solution is demonstrated by numerical experiments.

BEM-simulation of tubes using thin elements

Wolfgang Kreuzer (*Austrian Academy of Sciences, Austria*)

09:10

Veronika Weber (*Austrian Academy of Sciences, Austria*)

The simulation of the acoustic of tubes and pipes has been of interest for some time now, and applications range from musical instruments to the simulation of exhaust tubes. The "classical" theory for pipes assumes that the radius/wavelength ratio is small enough to ensure plane wave propagation, and the first resonance of the pipe can be determined by using the length of the pipe plus a correction factor dependent on the radius of the tube/pipe.

In this talk, we want to look at a simple BEM model of a musical tube (boomwhackers, Klangröhre, sound tube) that is a toy for children made of plastic. Although the example used here is a straight tube the advantage in the BEM formulation lies in the fact that non-straight tubes lined with different materials can be simulated rather easily. The length of the thin tubes (about 1mm wall width) range from 30.5 cm to approximately 63 cm, with a radius of 1.75 cm ranging from the notes C5 (ca. 538Hz) to C4 (ca. 262 Hz). In contrast to most FEM/BEM models for pipes the walls of the pipe are modelled using special thin elements. This setup has the advantage that we do not have to distinguish between exterior and interior domains, and that there is no need for special boundary conditions at the end of the tubes. In fact, the whole system can be modelled as an exterior problem. For the numerical experiments in this study we assume the tube walls to be sound hard, the excitation force is either given by a velocity boundary condition or by a point source inside the tube. We investigate the performance of these elements and the influence of the mesh size on the results by looking on the expected, measured and calculated resonance frequencies.

S12.04 | Waves and acoustics

Date: February 20, 2019

14:00-16:00

Room: HS 34

Cabin noise prediction using wave-resolving aircraft models

Sabine Christine Langer (*Technische Universität Braunschweig, Germany*)

14:00

Christopher Blech (*Technische Universität Braunschweig, Germany*)

Within the Coordinated Research Centre (CRC) 880, future civil aircraft with short take-off and landing capabilities are investigated. A main motivation are efficient point-to-point connections within Europe. Environmental friendliness is a key factor in the development of such aircraft systems in order to ensure the acceptance of new technologies. Therefore, the sound immission at the ground and in the passenger cabin is a major focus in the project. In this paper, wave-resolving models of complex aircraft fuselage structures and solution strategies of these large systems in frequency domain are presented.

On the basis of preliminary aircraft design data available in the project, a mechanical model of all fluid and structural parts is developed. The model comprises the back partition starting from the wing-box and assumes a linear behaviour in deflection, strain and material. The thickness distribution on the outer surface, the stiffeners, the floor, the bulk heads and the inner panels are considered concerning the structural domain. The insulation is modelled by an equivalent fluid approach. The cabin fluid, the structural domain, and the insulation are fully coupled. All domains are discretised automatically applying coincident nodes at the coupling interfaces. Frequency-dependent pressure fluctuations distributed on the outer surface as a result of Computational Aeroacoustic (CAA) simulations of jet noise are applied to the model. A realistic

consideration of such characteristic noise footprints is only possible due to the wave-resolving approach. The direct result of the aircraft model is the cabin's pressure field in frequency domain. The finite element discretisation leads to a system of equations with 1-3 mio degrees of freedom to be solved in frequency domain. As one solver run is easily realised, many solutions in the frame of uncertainty analyses or sensitivity studies require an highly efficient solution process. Different strategies applying direct solvers, iterative solvers or its combination are discussed within this contribution as well.

High-order shape functions for interior acoustics

Fabian Duvigneau (*Otto-von-Guericke-University Magdeburg, Germany*)

14:40

Sascha Duczak (*Otto-von-Guericke-University Magdeburg, Germany*)

The acoustic behavior of structures has lately been in the focus of industrial applications, due to the fact that the acoustic emission of a product is one major parameter which significantly influences the customer perception with respect to comfort and functionality. In this context, the numerical simulation of vibroacoustic problems needs to provide reliable information in order to be able to evaluate the acoustic behavior of new products already in an early stage of the product development process. With the help of a suitable simulation model expensive experimental studies can be reduced and acoustically improved designs can be developed. However, there are already commercial software tools available which offer the opportunity to solve coupled vibroacoustic problems. These tools are typically based on conventional low-order finite element methods (h-FEM) for solving the governing partial differential equations (PDEs) of the problem. In this contribution the advantages of high-order finite element methods, such as a possibly exponential convergence rate, will be exploited. In such an approach the same accuracy can be obtained by using significantly less degrees of freedom (dof) compared to classical h-FEM simulations. Consequently, the required computational time required for the analysis can be significantly reduced for a given target accuracy. This property is of special importance when complex structures of practical relevance are under investigation. Even today the overall efficiency of the simulation process is still an issue, despite the ever growing computational power. To exploit the described advantages, high-order FEMs have to be extended to acoustical problems. The advantage of high-order methods has been demonstrated by the authors in previous studies, e.g. in the context of wave propagation analysis and multi-physics applications such as piezoelectricity. In this contribution the developed high-order simulation approach is discussed and the received results are compared with commercial finite element solutions. Here, the focus is placed on the accuracy and the required computational effort of the different methods.

Infinite elements for exterior Helmholtz resonance problems based on a frequency dependent complex scaling

Lothar Nannen (*TU Wien, Austria*)

15:00

Markus Wess (*TU Wien, Austria*)

Complex scaling is a popular method for treating scattering and resonance problems in open domains. Thereby the unbounded domain is decomposed into a bounded interior and an unbounded exterior part. Subsequently, complex scaling is applied to the exterior domain to obtain exponentially decreasing solutions. Afterwards the complex scaled exterior is usually truncated and discretized using finite elements. To avoid truncation and obtain a better approximation we use infinite elements, which are based on Hardy space infinite Elements.

For solving scattering problems it is common to use frequency dependent scaling functions, whereas for treating resonance problems usually frequency independent scalings are applied to conserve the linearity of the resulting eigenvalue problem. Unfortunately a frequency independent

complex scaling works well only for a very narrow range of frequencies and the approximation depends heavily on the specific choice of the scaling function. To overcome this we use frequency dependent scaling functions for resonance problems as well, which leads to polynomial eigenvalue problems. The latter can be treated with no significant extra effort compared to linear problems by using a version of the shift-and-invert Arnoldi algorithm.

Absorbing boundary conditions for nonlinear acoustics: the Westervelt equation

Barbara Kaltenbacher (*Alpen-Adria-Universität Klagenfurt, Austria*)

15:20

Igor Shevchenko (*Imperial College, UK*)

We consider the Westervelt equation in an unbounded domain and propose nonlinear absorbing boundary conditions for its efficient and robust numerical simulations. We use the theory of pseudo- and para-differential operators as well as asymptotic expansions to derive local in space and time absorbing boundary conditions of low to high orders in a consistent way. The numerical studies demonstrate both the efficiency and effectiveness of the developed boundary conditions for different regimes of wave propagation in a wide range of excitation frequencies and angles of incidence.

Extension of the method of generalized ray to sound propagation in a wedge-shaped layer of fluid over a slow-speed elastic bottom

Piotr Borejko (*TU Wien, Austria*)

15:40

Objectives of author's research work on the three-dimensional (3-D) propagation of sound in shoal water are outlined in this abstract.

In sloping-bottom configurations (as, for example, on the continental shelf) the propagation of sound may proceed along 3-D ray paths, since the change in both the plane of incidence and the incidence angle upon each bottom reflection introduces a curvature into the projection of a ray path onto the sea surface.

A benchmark model to investigate the 3-D sound in such configurations is that of an acoustic wave in a wedge-shaped layer of fluid overlaying a fluid or an elastic half-space, known as the penetrable wedge.

No exact solution has ever been found for acoustic waves generated by a point source in a penetrable wedge. The only solution, which is exact other than the omission of wave diffracted at the wedge apex, is that obtained by modifying the method of generalized ray for parallel layers. In the article published in 1989 Pao, Ziegler, and Wang formulated such a solution and computed the 3-D acoustic waves in a wedge of fluid overlaying a fluid-type bottom (the sea over a saturated sandy sediment).

The bottom has a major effect on the propagation of sound in shallow-water areas; thus modeling elasticity in the bottom is also important. The article by Pao, Ziegler, and Wang formed the basis for the later extension of their solution (the articles by Borejko, Chen, and Pao published in 2001 and 2018) directed at benchmark modeling of the 3-D sound on a continental shelf with an elastic-type bottom, such as a sediment possessing enough rigidity to transmit shear waves or an exposed rock.

Only recently the author applied the extended solution to accurately model the 3-D sound on a continental shelf when the shear wave speed in the bottom is slower than (but comparable to) the sound speed in the water. The numerical evaluation of the solution required a very careful treatment of the branch points due to the three wave speeds of the model, but also of the Scholte pole, since at low frequencies the contribution of Scholte interface wave may dominate.

S12.05 | Waves and acoustics

Date: February 20, 2019

16:30-18:30

Room: HS 34

Comparison of different models for stress singularities in higher order finite element methods for elastic waves

Jannis Bulling (*Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*) 16:30

Hauke Gravenkamp (*University of Duisburg-Essen, Germany*)

The Spectral Element Method (SEM) has been proven to be an efficient numerical method for solving the wave equation in linear elastic bodies. This efficiency is reduced if a stress singularity is present in the body. For example, re-entrant corners, material interfaces, fixed boundaries, and especially crack tips can cause stress singularities. To preserve the efficiency of the SEM, special solution strategies are required. There are many approaches which consider stress singularities, but comparisons are rare for dynamic problems. Finding an efficient model is an important step for many applications. In particular, applications for structural health monitoring and non-destructive evaluation rely on accurate and efficient crack models.

In this contribution, we present several models to capture singularities in combination with the SEM. The theory behind the models are shortly summarized and we show results for different benchmark problems in two dimensions. The first model deploys a new class of singular elements. For these singular elements, the crack tip approximation is computed based on the static Scaled Boundary Finite Element Method (SBFEM). The second model uses the continued-fraction-based SBFEM, while the third model uses an hp-refinement near the singularity. The models are compared among each other and evaluated in terms of their respective efficiency and accuracy.

Spectral super elements for beams with arbitrary cross section

Axel Greim (*Technical University of Munich, Germany*) 16:50

Gerhard Müller (*Technical University of Munich, Germany*)

Spectral Super Elements are semi-analytical elements for the calculation of the wave propagation in structures with a constant cross section. They base on a finite element discretization in the cross-sectional directions and wave functions as ansatz for the longitudinal direction. No discretization in the latter direction has to be carried out and therefore the number of degrees of freedom is independent of the length the structure.

The wave functions used as ansatz are gained as eigenvalues (wave numbers) and -vectors (wave forms) from the quadratic eigenvalue problem of the infinite structure (in longitudinal direction). The infinite structure is reduced to a 2D problem with the help of a Fourier transformation in longitudinal direction. This method is called Waveguide Finite Element Method or 2,5D-Finite Element Method in literature. Thereby, the number of gained wave functions is two times the number of cross-sectional degrees of freedom.

In this study we compare the performance of Spectral Super Elements for beams with arbitrary cross sections with analytical solutions for the Euler Bernoulli Beam at low frequencies and with results form a 3D Finite Element analysis with commercial software for higher frequencies. We focus on numerical issues of the Spectral Super Elements and suggest procedures for the selection of wave functions form the full set for the ansatz in longitudinal direction.

Intersection of two elastic waves in the region of material nonlinearity in an elastic layer

Yanzheng Wang (*University of Siegen, Germany, Zhejiang University, China*)

17:10

Weiqliu Chen (*Zhejiang University, China*)

Chuanzeng Zhang (*University of Siegen, Germany*)

The intersection of two SH waves of lowest modes with a local cylindrical region of quadratic material nonlinearity in an elastic layer is investigated. For the cylindrical region, the nonlinear governing equations and the nonlinear boundary conditions are reduced to a set of linear equations at different orders by making use of the perturbation method. The SH waves of lowest modes satisfy the zero-order equations. At the first order, a series of inhomogeneous equations are obtained by substitution of the expressions of the SH waves into the nonlinear terms, which have the same forms as the equations governing the forced wave motion in an elastic layer. Mathematically, the first-order equations can be solved in a similar way when the inhomogeneous terms are viewed as the equivalent body forces and surface tractions. Based on the mode expansions, the amplitudes of the Lamb wave and the SH wave generated by the equivalent body forces and the surface tractions are obtained by using the reciprocity relation. It is of interest to note that only the coefficient of the lowest mode is nonzero for the generated SH wave. Numerical examples are presented for the scattered Lamb wave of zero-order mode and the SH wave propagating in a thin elastic layer. Based on the results, the methods to optimize the measurements or detections are proposed for the nonlinear nondestructive evaluation and test.

Numerical study of nonlinear elastic wave propagation in locally damaged engineering structures

Benjamin Ankay (*University of Siegen, Germany*)

17:30

Chuanzeng Zhang (*University of Siegen, Germany*)

Today's buildings and infrastructures are often exposed to severe external influences like mechanical over-loading, cyclic loading and corrosion, which may lead to a progressive development of the damage in certain localized areas of these structures. In engineering structures, the early damage stage is usually characterized by an increasing micro-damage, leading to a change in the nonlinear elastic material behavior and wave attenuation in these structures. In addition to the classical nonlinear elasticity theory, a pronounced hysteretic material behavior may also contribute to the overall material nonlinearity. In the case of an early damage detection in engineering materials, nonlinear ultrasonics has been proven to be a quite sensitive and effective nondestructive testing method. This method is based on an evaluation of the higher-order harmonics content in the frequency spectrum of the corresponding ultrasonic signals. To study the nonlinear ultrasonic wave propagation phenomena in classical and nonclassical nonlinear elastic medium, numerical simulations are of particular importance.

In this paper, the two-dimensional (2-D) ultrasonic wave propagation problem in an elastic half-space with a localized damaged zone is numerically simulated by a mapped Chebyshev pseudo-spectral method [1]. The considered damaged zone, which is embedded in an undamaged host medium, is modelled by a nonlinear elastic and viscoelastic constitutive law. Classical nonlinear elastic and nonclassical hysteretic material behaviors are separately considered and evaluated. In particular, the classical nonlinear elasticity theory of Murnaghan [2] is implemented, while the hysteretic material behavior is modelled by the Duhem-model. To transfer the constitutive relations from the one-dimensional (1-D) to the 2-D case the Kelvin decomposition method is used. Furthermore, Convolutional Perfectly Matched Layers (CPML's) are used to simulate the semi-infinite elastic half-space. The received time-domain signals are transformed to the

frequency-domain and subsequently analyzed for different degrees of the wave attenuation and nonlinearity in the damaged zone. The applications of the nonlinear ultrasonic technique are discussed based on the numerical results.

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An analytical approach for assessing wave scattering by pipelines in irregularly compacted soil

Wolfgang E. Weber (*Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg, Germany*) 17:50

George D. Manolis (*Aristotle University of Thessaloniki, Greece*)

There are many regions worldwide experiencing earthquakes which may lead serious damage in their infrastructures, e.g., buried infrastructure such as pipelines, tunnels, etc. As an example, such earthquakes may cause small landslides which successively lead to loose soil around those buried structures. As a consequence, high bending stresses may develop around their circumference and/or their length, causing breakage and other modes of failure. In the case of oil spilling out of a pipeline, this negatively affects the environment and additionally produces huge financial loss. There is nowadays high interest in automatically detecting where such leakages due to loose soil may occur. One method towards achieving this goal is based on the use of the principles of elastic wave propagation. Therefore, shakers and similar equipment is used to initiate elastic waves, which propagate through the soil and which are scattered by the pipeline. The measured scattered wave field is evaluated to gain insights into the current state of the soil surrounding the respective buried structure. Once loose soil is detected around the pipeline, then corrective measures can be taken such as systematic soil re-compaction.

In this contribution, an analytical approach is introduced which allows for modelling the elastic wave propagation through a Biot-type material such as soft soils. The approach focuses on time-harmonic SH-waves and includes the modelling of an irregularly compacted region around the pipeline. It is shown that the wave field scattered by irregularly compacted soil can be clearly distinguished from the wave field scattered by regularly compacted soil.

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Green's function for a horizontally layered anisotropic soil

Holger Waubke (*Austrian Academy of Sciences, Austria*) 18:10

Wolfgang Kreuzer (*Austrian Academy of Sciences, Austria*)

Tomasz Hrycak (*Austrian Academy of Sciences, Austria*)

Sebastian Schmutzhard (*Austrian Academy of Sciences, Austria*)

The Green's function for an anisotropic horizontally layered soil can be determined in the wave-number frequency domain. Only the vertical axis remains in the original domain. For a simulation in 2.5D a numerical inverse Fourier integral transformation, about one horizontal axis is needed. This leads to difficulties at the singularities of the function. For the boundary element method in 2.5D the integrals along the boundary are transformed to the wave-number domain

and solved analytically. The result is a filter that attenuates the spectrum of the Green's function and therefore allows for an inverse Fourier transformation using numerical methods. For an efficient inverse transformation the Filon method together with an adaptive algorithm are used.

S12.06 | Waves and acoustics

Date: February 21, 2019
Room: HS 34

08:30-10:30

Steady transonic dense gas flow past compression/expansion ramps revisited

Alfred Kluwick (*Technische Universität Wien, Austria*)
Ted Cox (*University College Dublin, Ireland*)

08:30

Supersonic flow past compression/expansion ramps represents a canonical problem in fluid dynamics which has been studied extensively in the past assuming perfect gas behaviour. More recently real gas effects on such flows have received increasing attention as part of efforts to, among others, increase the efficiency of Organic Rankine Cycles for decentralized power plants. Of special interest in this connection are dense gases of Bethe - Zel'dovich - Thompson fluids which have the distinguishing property that the so called fundamental derivative of gasdynamics $\Gamma = 1/c\delta(c\rho)/\delta\rho$ takes on negative values in the general neighbourhood of the thermodynamic critical point. Asymptotic analysis of the transonic flow regime has so far concentrated on cases where the unperturbed state with pressure p_0 , density ρ_0 and entropy s_0 is close to the transition curve $\Gamma = 0$ in the pressure, specific volume plane $(p, 1/\rho)$ such that $\Gamma_0 \ll 1, \Lambda_0 = \delta\Gamma/\delta\rho = O(1)$, Kluwick and Cox (2017, 2018). These studies have revealed a number of new phenomena and a non-uniqueness of solutions with a multiplicity exceeding that known from the theory of perfect gases.

Here we extend the analysis to cover flows where the unperturbed state in the $p, 1/\rho$ plane is in the vicinity of the point on the transition line where Γ and Λ vanish simultaneously. Such flows have $\Gamma_0 \ll 1, \Lambda_0 \ll 1, N_0 = \delta^2\Gamma/\delta\rho^2 = O(1)$ and are of considerable practical interest as isentropes that can be realized experimentally at present just barely enter the negative Γ region. Again an increased variety of possible solutions is observed.

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Multiple scales analysis of the undular hydraulic jump over horizontal surfaces

Dominik Murschenhofer (*TU Wien, Austria*)
Wilhelm Schneider (*TU Wien, Austria*)

08:50

The undular hydraulic jump is a peculiar but well known event occurring in slightly supercritical free-surface flows, characterized by a wavy surface shape with slowly changing amplitude and wavelength. For the present investigation stationary turbulent open-channel flow over a horizontal bottom is considered. The basic equations are the continuity equation for incompressible flow and the Navier-Stokes equations with Reynolds stresses (the so-called Reynolds equations). Kinematic and dynamic boundary conditions at the free surface are prescribed. Written in non-dimensional form, the basic equations contain two non-dimensional parameters, namely the Froude number Fr and a "friction Froude number" Fr_τ , which is defined in terms of the friction

velocity u_τ . A multiple scales analysis is applied to the governing Reynolds equations in the double limit of Froude numbers approaching the critical value 1, i.e. $Fr = 1 + (3/2)\epsilon$ with $\epsilon \rightarrow 0$, and very small friction Froude numbers, i.e. $Fr_\tau \rightarrow 0$, which is equivalent to very large Reynolds numbers. Coupling the two small parameters according to $Fr_\tau^2 = B\epsilon^3$ with the constant coupling parameter $B = O(1)$ allows to perform the analysis without the use of any turbulence modeling or empirical parameters. First, a multiple scaling solution for the first-order perturbation $H_1(X)$ of the surface elevation is found, with X denoting the contracted longitudinal coordinate. Secondly, it is shown that

$$H_1'''' + H_1'(H_1 - 1) + \gamma = 0, \quad \text{with} \quad \gamma = \epsilon^{1/2}B/9,$$

is a uniformly valid ordinary differential equation for $H_1(X)$. Equation (1) represents a steady-state version of the Korteweg - de Vries equation, extended by a constant damping term γ . The analytical solutions of the multiple scales analysis are compared with numerical solutions of Eq. (1), as well as with experimental data for horizontal bottoms. In addition, solutions according to a previously published theory for undular hydraulic jumps over inclined bottoms are also discussed.

Growth and decay of waves in countercurrent air-water turbulent flows

Francesco Zonta (*TU Wien, Austria*)

09:10

Miguel Onorato (*University of Torino, Italy*)

Alfredo Soldati (*TU Wien, Austria*)

Mass, momentum and energy transport phenomena through a deformable air-water interface are important in many geophysical processes and industrial applications. In this study we use Direct Numerical Simulations (DNS) to explore the dynamics of a countercurrent air/water flow. The motion of the air/water interface is computed by solving an advection equation for the interface vertical elevation (boundary fitted method). At each time step, the physical domain is mapped into a rectangular domain using a nonorthogonal transformation. Continuity and Navier-Stokes equations are first solved separately in each domain, then coupled (velocity/stress) at the interface. DNS are performed in the Weber, Froude and Reynolds number (We, Fr, Re) parameter space.

Regardless of Re, Fr and We, the process of wave generation is initially driven by surface tension and follows a universal scaling $t^{2/5}$. Later in time, the growth rate of waves depends on the value of Fr, We: for small capillary waves, we do not observe substantial changes from the $t^{2/5}$ law; for larger and longer waves (for which gravity is not negligible) we observe a faster growth rate. After the transient evolution, the interface deformation reached a statistically steady state that we characterize by measuring the wavenumber spectra of the interface deformation. We found a good agreement between our results and those given by Wave Turbulence Theory. We also compute and discuss the wave-induced modification of the average wind (air) and current (water) velocity profiles.

When the applied wind is reduced or removed, waves decay exponentially towards a new asymptotic state (which takes the form of a flat interface if the wind is completely removed). The parameters characterizing this exponential decay do depend on the specific value of Re, Fr, We. We finally derive simple phenomenological models to explain our results for both wave growth and decay.

Stationary single waves in turbulent free-surface flows

Mario Stojanovic (*TU Wien, Austria*)

09:30

Wilhelm Schneider (*TU Wien, Austria*)

Dominik Murschenhofer (*TU Wien, Austria*)

The comparison between asymptotic analysis and numerical computations is of great interest, especially if experimental data is provided. Thus, one can get an idea about the influence of the assumptions that were made during the computations.

In this talk a steady turbulent near-critical free-surface channel flow is considered, whose stationary waveform is of key interest. The roughness of the inclined bottom is allowed to vary with the space coordinate, such that the values of roughness are locally-enhanced in a certain region of the channel. The flow is assumed to be fully developed far upstream and far downstream.

In [1], an asymptotic analysis was performed for large Reynolds numbers and Froude numbers close to the critical value 1, leading to the steady-state version of an extended Korteweg-de Vries (KdV) equation. The solution of this ODE yields the first-order perturbation for the surface elevation.

For the numerical approach the full equations of motion are solved with the help of a CFD-program using a standard turbulence model. In order to obtain the shape of the free surface an iteration procedure is used, which was successfully applied to the related problem of the undular hydraulic jump [2]. This iteration procedure is based on a further asymptotic expansion, which leads to an additional term in the extended KdV equation. This term allows to correct the surface elevation successively, starting from a solution of the nonlinear ODE which was derived in [1].

Besides the solitary wave, the so-called single wave of the second kind is studied numerically. The shape of the single wave of the second kind differs from the shape of the well-known solitary wave in terms of amplitude and the decay behaviour upstream as well as downstream. Its existence was predicted recently [3].

The numerical results are compared with theoretical predictions and experimental data [4].

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Analysis of sound generation of sub- and super-sonic boundary layer flows

Yi Zhang (TU Darmstadt, Germany)

09:50

Martin Oberlack (TU Darmstadt, Germany)

The theory of acoustics is based on the linearized Euler equations for compressible flows. For plane shear flows, a normal-mode approach for density, pressure and velocity is applied, similar to the classical stability theory, which involves Fourier decomposition of the disturbances into main flow direction, span and time. The Pridmore-Brown equation results, a second order equation, whose complexity is depending on the ansatz of the velocity profile. Before our study, there were only analytical solutions for the simplest case, i.e. the equation with a linear shear profile, since the complete solution of other velocity profiles turned out to be difficult due to various mathematical obstacles.

In our approach, we first study the analytical solution of the two-dimensional Pridmore-Brown equation for a boundary layer flow, where the velocity profile is approximated by an exponential. With this, the Pridmore-Brown equation can be solved in terms of the confluent Heun function (CHF), which is a solution of the confluent Heun equation (CHE) introduced by K. Heun in 1888, a generalization of the hypergeometric equation.

Next, together with the appropriate boundary conditions, i.e. the acoustic perturbation vanishing at infinity and the acoustic analogue of an impermeable wall, the boundary value problem is converted to an algebraic eigenvalue problem, where the Mach and the wave number are free parameters and the frequency is the eigenvalue. Based on this we analyze the behavior of the eigenvalue problem. In the limit of small wave numbers, the resulting frequency is unique and real-valued. In the limit of large wave numbers, the eigenvalues are not only multiple but also

involve imaginary parts. The above analytical results are validated by numerical methods. It is to be concluded that the existence of an imaginary part of frequency indicates towards an acoustic instability of the exponential boundary layer.

Furthermore, to investigate the more general character of the frequency-eigenvalues, we determine the upper (UL) and lower (LL) limit of the eigenvalues as functions of the Mach-number. The start points on the UL explains well the increase of multiple eigenvalues as wave number increases, which allow us to predict the number of the multiple eigenvalues corresponding to each wave number accurately. The UL and LL of the eigenvalue can besides numerical computations be validated by the asymptotic behavior in the limit of the large wave number.

Advanced finite element formulation for viscothermal acoustics

Manfred Kaltenbacher (*TU Wien, Austria*)

10:10

Florian Toth (*TU Wien, Austria*)

Hamideh Hassanpour Guilvaiee (*TU Wien, Austria*)

Sound waves in the vicinity to solid bodies are subjected to losses due to fluid viscosity and heat exchange. Thereby, we can define a viscous and thermal boundary layer, where these losses are relevant and have to be modelled. An efficient model is the use of an acoustic impedance condition and describing the sound field in the domain by the lossless wave equation. However, in MEMS (Micro-Electro-Mechanical-System) devices, domains or some part of it exhibit dimensions, which are similar to the boundary layer thickness, and so a description taking the losses in the domain into account is necessary. Such a description is provided by the time harmonic version of the linearized compressible flow equations (conservation of mass, momentum, energy and corresponding constitutive relations). Finally, three equations for the acoustic particle velocity, acoustic pressure and temperature are obtained. For the efficient numerical computation we apply the Finite Element (FE) method. Since viscothermal acoustics describe nearly an incompressible physical field, we apply Taylor Hood elements to obtain a stable and consistent FE formulation for the acoustic particle velocity (P2-, Q2-elements) and pressure (P1-, Q1-elements). Furthermore, since the two boundary layers are of similar thickness, we also apply second order basis functions for the temperature.

S12.07 | Waves and acoustics

Date: February 21, 2019

14:00-16:00

Room: HS 34

Towards an efficient direct noise computation of hydrodynamic-acoustic feedback mechanisms

Daniel Kempf (*University of Stuttgart, Germany*)

14:00

Thomas Kuhn (*University of Stuttgart, Germany*)

Claus-Dieter Munz (*University of Stuttgart, Germany*)

Direct noise computation (DNC) offers numerous advantages compared to hybrid approaches in simulating aeroacoustic mechanisms. In DNC, hydrodynamics and acoustics are solved in a coupled manner which allows to depict intricate interactions between both fields. However, this approach intrinsically requires the resolution of the disparate length and time-scales of nonlinear turbulent production and the acoustic propagation. Our open-source Discontinuous Galerkin (DG) framework FLEXI, has been successfully applied to this multiscale problem by predicting acoustic feedback loops e.g. of a side view mirror.

The first part of the talk has its focus on aeroacoustic feedback within cavities. Tonal cavity noise results from the interaction of the upstream boundary layer and the cavity. Here, the

incoming boundary layer is turbulent. Due to the high computational cost of resolving most of the turbulent scales, the simulated part of the setup needs to be zonal around the cavity. This zonal LES approach requires a turbulent inflow condition which has good properties both in terms of acoustic as well as the turbulent boundary layer characteristics. In this talk we will present an implementation for DG of the anisotropic linear forcing by de Laage de Meux. To further reduce computational cost, a wall model has been implemented and its impact on cavity acoustics has been analyzed. The whole zonal LES approach is then applied to open cavity simulations which are validated against wind tunnel experiments.

Despite the high efficiency of the framework, the aim of the second part of the talk is to draw the attention to an efficient method for the detection of aeroacoustic feedback. The occurrence of aeroacoustic feedback can be effectively predicted with a global stability analysis. Here, an impulse response analysis on a time averaged flow field is carried out. The underlying baseflow is maintained constant through volume forcing terms. This method was successfully applied by Frank to prove the existence of acoustic feedback on a side view mirror.

To overcome the drawback of computationally expensive long time-averaging, the question arises if a computationally less expensive numerical method, ideally a RANS-solver, can be employed to generate the time-averaged baseflow. Results of a simplified side view mirror will demonstrate the advantages of the latter approach.

In summary, this lecture will introduce different methods to depict aeroacoustic feedback with our high-order framework FLEXI. The focus is on increasing the efficiency in order to facilitate future industrial use.

Helmholtz decomposition of compressible flow data at Mach 0.8

Stefan Schoder (*TU Wien, Austria*)

14:40

Clemens Freidhager (*TU Wien, Austria*)

Manfred Kaltenbacher (*TU Wien, Austria*)

The Helmholtz decomposition separates a compressible velocity field into vortical and compressible structures. Based on the compressible flow simulation, we show the Helmholtz decomposition $u = u^v + u^c = \nabla \times A^v + \nabla \phi^c$ (1), of a compressible flow field over a rectangular cavity at Mach 0.8. In (1), u^v represents the solenoidal (vortical) part and u^c the irrotational (compressible) part. This contribution motivates the decomposition as a powerful tool during the postprocessing of direct aeroacoustic simulations. In particular, we discuss the vector-potential formulation $\nabla \times \nabla \times A^v = \nabla \times u$, of the Helmholtz's decomposition and present the superiority of the vector formulation over the scalar formulation. The formulation has been implemented in the finite element software CFS++ [1] and is applied to the rectangular cavity at Mach 0.8.

References:

[1] M. Kaltenbacher. Numerical Simulation of Mechatronic Sensors and Actuators: Finite Elements for Computational Multiphysics, 3rd Edition. Springer (2015)

Uncertainty quantification for direct noise computation of cavity feedback

Thomas Kuhn (*University of Stuttgart, Germany*)

15:00

Noise emitted by flow over cavities has in recent years become a major concern in automobile exterior aerodynamics. Different noise generation mechanisms have been identified in cavities, such as Helmholtz resonance and Rossiter feedback, which can both lead to tonal noise. Rossiter feedback is characterized by a two-way interaction between aeroacoustics and hydrodynamics. This necessitates the use of direct noise computation, where acoustic sources are directly resolved in a compressible LES (as opposed to hybrid simulations, where hydrodynamics and aeroacoustics are treated in two consecutive steps). To achieve the necessary multi-scale resolution and low

numerical dissipation, a high-order method is advantageous. Both frequencies and noise levels are highly sensitive to the simulation setup. The dominant acoustic modes can switch abruptly. Applying uncertainty quantification (UQ) to the problem setup is therefore a promising way to gain a more complete insight into the factors influencing the generated noise spectra. In UQ, uncertain input parameters (here, for example, uncertain inflow conditions and cavity geometry) are treated as random variables.

Our deterministic simulations are carried out using a discontinuous Galerkin spectral element method. Turbulence is generated with a volume forcing term based procedure at the inflow. To quantify the impact of uncertainty on aeroacoustics, we have implemented a non-intrusive spectral projection method.

The talk will start with a brief overview of the numerical framework and give some insight into algorithmic and implementational aspects. In a second part of the talk this UQ-DG framework is applied to open cavity simulations. We start with results from 2D cavity simulations with a laminar upstream boundary layer. We demonstrate the impact of uncertain input like the cavity length or depth and the boundary layer thickness on Rossiter feedback, which results in non-linear effects such as mode-switching. Building on those results, we further present 3D open cavity simulations with an upstream turbulent boundary layer. Here, we can analyze not only the uncertain parameters applied to the 2D DNS simulations but also the uncertain impact of the turbulent modelling approaches on cavity noise. We conclude the talk by pointing out how the application of UQ to aeroacoustic simulations helps to get a deeper understanding of cavity noise generation mechanisms.

Numerical investigation of the resonance behavior of flow-excited Helmholtz resonators

Michael Weitz (*TU Wien, Austria*)

15:20

Stefan Schoder (*TU Wien, Austria*)

Manfred Kaltenbacher (*TU Wien, Austria*)

The turbulent flow over mirrors and functional gaps of cars poses a relevant sound source in automotive acoustics and has a great influence on the noise level inside the car cabin. These gaps combined with the underlying volume of air represent Helmholtz resonators that are excited at their resonance frequency by the turbulent flow.

Based on models that describe the spatial correlation of pressure fluctuations beneath a turbulent boundary layer (e.g. Corcos model) we present how to compute an extensive synthetic excitation signal that shows the desired correlation properties. Moreover, this contribution shows the capabilities of complex fluid models to better predict the resonance behavior of Helmholtz resonators. Finally, an acoustic simulation is presented, where both the synthetic excitation signal and the complex fluid model are applied, using CFS++.

Numerical calculation of aerodynamic noise generated from missile in low mach number flight

Bosko Rasuo (*University of Belgrade, Serbia*)

15:40

Vladimir Jazarevic (*University of Belgrade, Serbia*)

Paper describes numerical prediction of aerodynamic noise generated from the missile. Simulation of turbulent flow is done solving incompressible Navier-Stokes equation, where turbulence is modelled with the orthogonal subgrid scale (OSGS) method with dynamical subscales. Because of comparison, the same simulation is done using the LES (Large Eddy simulation). It is shown how simulation of turbulent flow affects the prediction of acoustic sources calculated using Lighthill's analogy. Translation from time to frequency domain is done through DFT (Direct Fourier

Transform), which gives smaller usage of memory. Acoustic sources are used in inhomogeneous Helmholtz equation to simulate pressure wave propagation in the domain. It is shown that OSGS with dynamical subscales gives better representation of the spectrum. Overall, better prediction of energy transfer across large and small eddies will give better allocation and presentation of acoustics sources. These sources will change wave propagation of the pressure in acoustic field.

S12.08 | Waves and acoustics

Date: February 22, 2019

08:30-10:30

Room: HS 34

A mesoscale material model to describe continuous mode conversion of lamb waves in composite materials

Eugen Zimmermann (*Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg, Germany*) 08:30

Artem Eremin (*Kuban State University, Krasnodar, Russia*)

Rolf Lammering (*Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg, Germany*)

The objective of the homogenisation of micro-heterogeneous materials within the framework of continuum mechanics is obvious: substitution of the heterogeneous microstructure by a homogeneous continuum on the macroscale. For this purpose, the effective properties are obtained using a representative volume element (RVE). For many engineering applications and research questions, the resulting homogeneous material model is sufficient to adequately represent the problem under consideration.

In certain situations, the macro scale is not suitable and it is necessary to introduce an intermediate scale also known as the mesoscale. The obtained material parameters on this scale are called apparent properties. For example, a phenomenon which can be described with these properties is the continuous mode conversion (CMC) which may take place in the course of Lamb wave propagation in composite plates. Lamb waves are guided waves travelling in thin-walled structures. In general, an infinite set of possible particle motions exists in plate like structures, but it is possible to categorize them into symmetric and asymmetric modes.

The CMC phenomenon is similar to the local mode conversion, which usually occurs in homogeneous materials in the presence of an inhomogeneity. If a symmetrical mode encounters a damage while propagating through the structure, then it converts in an asymmetric mode at an obstacle. The conversion is usually bound to the location of the obstacle. In contrast, CMC occurs in damage-free structures made of carbon fiber reinforced plastic and manifests itself as conversion takes place permanently or continuously. The reason for this phenomenon, beside the design of composite materials, is the inhomogeneous distribution of material parameters on the mesoscale, which is caused by the random fiber distribution.

The current work deals with the formulation of a material model on the mesoscale with random properties. The model is based on apparent properties, which are determined using a volume element smaller than the RVE. This results in a spatial fluctuation of the obtained material parameters. Furthermore, the averaging over a region smaller than the RVE means that the volume element cannot be regarded as representative. To handle this issue the microstructure is considered as a realization of an ensemble describing a random medium. For this purpose, the theory of random fields is applied to describe the material behaviour. As an example, the construction of a material based on a correlation model with scale dependent material parameters is presented, which at the end is used to reproduce CMC.

Dynamic anisotropy and localisation in relaxed micromorphic continua

Domenico Tallarico (*INSA-Lyon, France*)

08:50

Gabriele Barbagallo (*INSA-Lyon, France*)

Marco V. D'Agostino (*INSA-Lyon, France*)

Alexios Aivaliotis (*INSA-Lyon, France*)

Patrizio Neff (*University of Duisburg-Essen, Germany*)

Angela Madeo (*INSA-Lyon, France*)

In this talk, we show that transient waveforms arising from several localised pulses in a microstructured material can be reproduced by a corresponding generalised continuum of the relaxed micromorphic type. In the low frequency regime, the anisotropic waveforms are captured by an effective Cauchy theory. At higher frequencies, such as in the band-gap or for frequencies corresponding to the optical branches, localised waveforms are well reproduced by the relaxed micromorphic model.

Effective description of anisotropic wave dispersion in mechanical band-gap metamaterials via the relaxed micromorphic model

Angela Madeo (*INSA Lyon, France*)

09:10

The relaxed micromorphic material model for anisotropic elasticity is used to describe the dynamical behavior of a band-gap metamaterial with tetragonal symmetry. The proposed model is able to capture all the main microscopic and macroscopic characteristics of the targeted metamaterial, namely, stiffness, anisotropy, dispersion and band-gaps.

The simple structure of our material model, which simultaneously lives on a micro-, a meso- and a macroscopic scale, requires only the identification of a limited number of frequency-independent and thus truly constitutive parameters, valid for both static and wave-propagation analyses in the plane.

Microstructure-related Stoneley waves and wavefront manipulation at a 2D Cauchy/relaxed micromorphic interface

Alexios Aivaliotis (*INSA Lyon, France*)

09:30

Ali Daouadji (*INSA Lyon, France*)

Domenico Tallarico (*INSA Lyon, France*)

Marco Valerio d'Agostino (*INSA Lyon, France*)

Patrizio Neff (*Universität Duisburg-Essen, Germany*)

Angela Madeo (*INSA Lyon, France*)

In this paper we study the reflective properties of a 2D interface separating a homogeneous solid from a band-gap metamaterial by modeling it as an interface between a classical Cauchy continuum and a relaxed micromorphic medium. We show that the proposed model is able to predict the onset of Stoneley interface waves at the considered interface both at low and high-frequency regimes. More precisely, critical angles for the incident wave can be identified, beyond which classical Stoneley waves, as well as microstructure-related Stoneley waves appear. We show that this onset of Stoneley waves, both at low and high frequencies, strongly depends on the relative mechanical properties of the two media. We suggest that a suitable tailoring of the relative stiffnesses of the two media can be used to conceive “smart interfaces” giving rise to wide frequency bounds where total reflection or total transmission may occur.

Tuning of vibration and wave propagation characteristics in pre-deformed periodic lattice frame structures

Marius Mellmann (*University of Siegen, Germany*)

09:50

Chuanzeng Zhang (*University of Siegen, Germany*)

The design, optimization and application of periodic materials and structures, such as phononic crystals or structures, are receiving increasing attention in recent years. Phononic crystals or structures can manipulate the characteristics of the elastic and acoustic wave propagation [1]. Thus, it is feasible to create the so-called band-gaps, designating certain frequency ranges, in which the propagation of elastic or acoustic waves is prohibited [2]. Accordingly, such structures have many promising applications in sound and vibration insulation as well as wave filters. Other applications of phononic crystals or structures are for example waveguides, wave focusing and wave splitting devices.

In general, the elastic or acoustic wave propagation properties in phononic crystals or structures can be tuned by changing the topology, the density and the stiffness of their components or by adding local resonators. For periodic lattice frame structures, it is also possible to manipulate the vibration and elastic wave propagation properties by pre-deforming the structural members. In this study, the influences of the pre-deformations on the vibration and elastic wave propagation characteristics in periodic lattice frame structures are analyzed by considering a representative unit-cell. The influences of both the amplitude and the shape of the pre-deformations will be investigated. Numerical examples will be presented and discussed to explore the effects of the pre-deformations on the vibration and elastic wave propagation properties in periodic lattice frame structures.

References

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S13 | Flow control

Organiser: Wolfgang Schröder (*RWTH Aachen University, Germany*)
Bernd Noack (*Limsi, France*)

S13.01 | Flow control

Date: February 19, 2019
Room: SR 07

08:30-10:30

Machine learning of interpretable nonlinear models for unsteady flow physics

Steven L. Brunton (*University of Washington, Seattle, WA, USA*) 08:30
J. Nathan Kutz (*University of Washington, Seattle, WA, USA*)
Jean-Christophe Loiseau (*Laboratoire DynFluid, Arts et Metiers ParisTech, Paris, France*)
Bernd R. Noack (*Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingenieur, LIMSI-CNRS, Orsay, France*)

Accurate and efficient reduced-order models are essential to understand, predict, estimate, and control unsteady fluid flows. These models should ideally be generalizable, interpretable, and based on limited training data. This talk will explore the sparse identification of nonlinear dynamics (SINDy) approach to uncover interpretable models for unsteady flow physics. First, we will discuss how it is possible to enforce known constraints, such as energy conserving quadratic nonlinearities, to essentially “bake in” known physics. Next, we will demonstrate that higher-order nonlinearities can approximate the effect of truncated modes, resulting in more accurate models of lower order than Galerkin projection. Finally, we will discuss the use of intrinsic measurement coordinates to build nonlinear models, circumventing the well-known issue of continuous mode deformation associated with methods based on the proper orthogonal decomposition. This approach will be demonstrated on several relevant systems in fluid dynamics with low-dimensional dynamics.

Artificial intelligence control applied to drag reduction of the fluidic pinball

Guy Yoslan Cornejo Maceda (*LIMSI-CNRS, France*) 09:10
Bernd R. Noack (*LIMSI-CNRS, France, TU Braunschweig, Germany, TU Berlin, Germany, HIT Shenzhen, China*)
François Lusseyran (*LIMSI-CNRS, France*)
Marek Morzynski (*PUT, Poland*)
Nan Deng (*ENSTA ParisTech, France*)
Luc Pastur (*ENSTA ParisTech, France*)

Flow control is at the core of many engineering applications, such as drag reduction for land-, sea- and air-borne transportation, lift increase of airfoils, mixing enhancement of chemical reactions and efficiency increase for wind turbines and marine current power, just to name a few examples. In particular, feedback turbulence control is a key enabler for those technologies (Brunton & Noack, 2015 Appl. Mech. Rev. 67, 050801).

The challenges in control design are the associated high-dimensional dynamics, significant time-delays from actuation to sensing, strong nonlinearities and frequency crosstalk, making modeling and linear control theory often impractical. To address these challenges, a model-free, self-learning control strategy is developed building on corresponding experimental studies of the

authors. The control design is formulated as a regression problem and solved with powerful methods of machine learning / artificial intelligence.

Our machine learning control (MLC, Duriez et al. 2016 Springer) is based on genetic programming (GP), a biological inspired method that mimicks the Darwinian process of natural selection to learn the control law in an unsupervised way. MLC is applied to a direct numerical simulation of the fluidic pinball which is taken as a drag reduction benchmark. Here, three cylinders are centered on an equilateral triangle in a two dimensional flow. The flow is actuated by three independent cylinder rotations and monitored by 9 sensors downstream. The fluidic pinball is a simple configuration which shares nonlinear features of many reported actuated real flows such as bifurcations and frequency crosstalk. The goal is to reduce the parasitic drag power accounting for the actuation expenditure.

On the methodological side, we increase the GP learning rate by a factor of 5, for instance, by parameter optimization and removing redundant control laws.

On the physical side, we achieve 46% reduction of the net drag power comprising open-loop boat-tailing and closed-loop phasor control after testing only 1000 individuals. This reduction outperforms all other optimized symmetric actuations (like constant and periodic forcing). We expect significant performance improvements of MLC in future turbulence control experiments.

Control of chaotic systems by deep reinforcement learning

Michele Alessandro Bucci (*LIMSI-CNRS, Orsay, France*)

09:30

Onofrio Semeraro (*LIMSI-CNRS, Orsay, France*)

Alexandre Allauzen (*LIMSI-CNRS, Orsay, France*)

Laurent Cordier (*PPRIME-CNRS, Poitiers, France*)

Lionel Mathelin (*LIMSI-CNRS, Orsay, France*)

In recent years, research efforts have been devoted towards the effective applications of control theory to flows in different regimes [1]. In the first approaches, Linear Quadratic Gaussian (LQG) control was extensively used to damp first-order fluctuations. However, the LQG framework encounters strong limitations. The implementation of LQG requires knowledge about the Jacobian of the flow operator around a steady state, is limited to a quadratic object function and requires an a-priori assessment of the "color" of the noise for the Kalman estimation filter. Moreover, the employment of LQG has to be questioned for fully nonlinear flows when the dynamics is self-sustained, saturated and the steady solution is never observed. In principle, in these cases, following the nonlinear trajectory means to continuously change the structure of the Jacobian operator (change of geometry or boundary conditions) and/or the objective function within a finite time horizon. For circumventing these limitations, optimal control can be reformulated into a more general nonlinear framework, that leads to the Hamilton-Jacobi-Bellman equation, applied in principle for any quadratic objective function; within this framework, the only a-priori assessment is the definition of an instant reward as measure of the quality of an action in a certain state. The objective function is then defined as the expectation of the cumulative rewards in the limit of an infinite time horizon to be maximized, the so-called action-value. This function, which associates to each state of the system the value of the objective function, cannot be exactly determined in general; however, it can be approximated with Neural Networks. The combination of this approximation and nonlinear optimal control leads to a new framework referred to as Deep Reinforcement Learning (DRL) [2,3]. The recent successes of DRL motivate the implementation of this approach also in fluid dynamical systems. In this work, we consider the Kuramoto-Sivashinsky (KS) equation as study-case to test the capability of DRL to control chaotic dynamics. After a first step of learning, necessary to explore the action-state phase space, the neural networks are trained such that the value predicted by the Bellman's equation is maximized. In this sense, the resulting control policy is optimal. In the final contribution, we will analyze the control action in the KS phase-state for a physical interpretation.

[1] Kim and Bewley, *Annu. Rev. Fluid Mech* (2007) [2] Volodymyr et al., *Nature* 518.7540 (2015): 529. [3] Lillicrap et al., arXiv preprint arXiv:1509.02971 (2015)

Control of transient instabilities by order reduction on optimally time-dependent modes

Antoine Blanchard (*MIT, United States of America*)

09:50

Themistoklis Sapsis (*MIT, United States of America*)

Identification and control of transient instabilities in high-dimensional dynamical systems remain a challenge because transient (non-normal) growth cannot be captured by low-dimensional modal analysis. Here, we leverage the power of the optimally time-dependent (OTD) modes, a time-evolving set of orthonormal modes that capture directions in phase space associated with transient and persistent instabilities, to formulate a control law capable of suppressing transient and asymptotic growth around any fixed point of the governing equations. The control law is derived from a reduced-order system resulting from projecting the linearized dynamics onto the OTD modes, and enforces that the instantaneous growth of perturbations in the OTD-reduced tangent space be nil. We apply the proposed reduced-order control algorithm to infinite-dimensional fluid flows dominated by strong transient instabilities, and demonstrate unequivocal superiority of OTD control over classical modal control.

S13.02 | Flow control

Date: February 19, 2019

16:30-18:30

Room: SR 07

External acoustic control of the laminar boundary layer separation over a circular cylinder

Mathias Lemke (*Technische Universität Berlin, Germany*)

16:30

Vincenzo Citro (*Università degli Studi di Salerno, Italy*)

Jörn Sesterhenn (*Technische Universität Berlin, Germany*)

Flavio Giannetti (*Università degli Studi di Salerno, Italy*)

An adjoint-based approach for the external acoustic control of the laminar boundary layer separation over a circular cylinder is presented. Inspired by experimental studies, we numerically investigate the control of the flow field by using external acoustic actuators.

The aim of this work is to provide a general theoretical framework to identify an optimal acoustic forcing able to suppress the arising instability. The optimal position of the acoustic sources is also localized. The employed adjoint-based strategy provides an effective control able to suppress the oscillations of the boundary layer separation points and the von-Karman vortex street. For two symmetric actuator positions, the resulting forcing functions have to be anti-symmetric. They correspond to the occurring vortex shedding frequencies during the transition. We found also that the limits of the proposed approach are related to the limits of linear acoustics. The present results provide useful information about the physical mechanism able to suppress noise generation in the flow past bluff bodies.

Aerodynamic drag reduction using trapped vorticity flow control

Michael DeSalvo (*Georgia Institute of Technology, United States of America*)

17:10

Ari Glezer (*Georgia Institute of Technology, United States of America*)

The aerodynamic performance of a wind tunnel wing model (NACA 4415) is substantially improved below stall when the base flow is fully-attached (at low angles of attack) by fluidic modification of its “apparent” shape using controlled trapped vorticity concentrations near the surface. Hybrid actuation is effected through controlled interactions between arrays of surface-mounted low-power synthetic jet actuators (momentum coefficient $C_m @ 10^{-3}$) that are integrated with a passive obstruction of scale $O(0.01c)$ and the local cross flow. The jet actuation frequency [$St_{act} \sim O(10)$] is selected to be at least an order of magnitude higher than the characteristic unstable frequencies of the airfoil wake, thereby decoupling the actuation from the global instabilities of the base flow. Regulation of vorticity production, accumulation, and transport in the vicinity of a hybrid actuator effects significant changes in local surface pressure distributions. The actuations engenders a strong local low-pressure domain coupled with favorable pressure gradient upstream and increased pressure downstream of the actuator and thereby changes in the airfoil’s global drag and lift. It is shown that regulation of the trapped vorticity on the pressure side of the airfoil leads to a significant reduction in drag. For example, at Reynolds number $Re = 6.1 \cdot 10^5$ and angle of attack $a = 4$ trapped vorticity actuation leads to drag reduction of over 30% compared to the base airfoil with minimal penalty in lift. PIV measurements show the spatial variation in the distribution of vorticity concentrations and yield estimates of the corresponding changes in circulation. These findings are corroborated by measurements and analysis of the changes in momentum flux in the wake due to actuation.

Perimetric blowing at the rear of a bluff body: consequences on the wake dynamics and drag reduction

Manuel Lorite-Díez (*Universidad de Jaén, Spain*)

17:30

José Ignacio Jiménez-González (*Universidad de Jaén, Spain*)

Luc Pastur (*IMSIA - ENSTA ParisTech, France*)

Olivier Cadot (*University of Liverpool, UK*)

Carlos Martínez Bazán (*Universidad de Jaén, Spain*)

Permanent asymmetry and bistable dynamics of the turbulent wakes of symmetric square-back bodies are caused by a global instability reminiscent from a steady bifurcation of the laminar regime. The present work investigates how base blowing at different locations may affect the wake asymmetry, or control the global instability correspondingly to the obtained drag reduction. We have conducted experiments at IMSIA to study the effect of steady perimetric blowings on wake dynamics and drag reduction. Drag reduction is optimal when the gas is blown at the top and/or bottom slits. When the blowing flow rate is small, drag is reduced due to mass injection in the recirculation bubble. Drag reaches a minimum value, before increasing again at higher flow rates, due to an increasing injection of momentum in the wake.

When blowing is off, at the Reynolds numbers and ground clearance considered, the wake dynamics is bistable, characterized by random switches between left to right-deflected wakes. In the regime of injection, the drag reduction is correlated to the bubble increase while no main changes in the long time bistable dynamics are observed, even when blowing breaks the reflectional symmetry (i.e. blowing left or right handside). In the momentum regime, corresponding to drag increase, any blowing orientates permanently the wake asymmetry.

Harnessing the Kelvin-Helmholtz instability: feedback stabilization of an inviscid vortex sheet

Bartosz Protas (*McMaster University, Canada*)

17:50

Takashi Sakajo (*Kyoto University, Japan*)

In this investigation we use a simple model of the dynamics of an inviscid vortex sheet given by the Birkhoff-Rott equation to obtain fundamental insights about the potential for stabilization of

shear layers using feedback control. As actuation we consider two arrays of point sinks/sources located a certain distance above and below the vortex sheet and subject to the constraint that their mass fluxes separately add up to zero. First, we demonstrate using analytical computations that the Birkhoff-Rott equation linearized around the flat-sheet configuration is in fact controllable when the number of actuator pairs is sufficiently large relative to the number of discrete degrees of freedom present in the system, a result valid for generic actuator locations. Next we design a state-based LQR stabilization strategy where the key difficulty is the numerical solution of the Riccati equation in the presence of severe ill-conditioning resulting from the properties of the Birkhoff-Rott equation and the chosen form of actuation, an issue which is overcome by performing computations with a suitably increased arithmetic precision. Analysis of the linear closed-loop system reveals exponential decay of the perturbation energy and of the corresponding actuation energy in all cases. Computations performed for the nonlinear closed-loop system demonstrate that initial perturbations of nonnegligible amplitude can be effectively stabilized when a sufficient number of actuators is used. We also thoroughly analyze the sensitivity of the closed-loop stabilization strategies to the variation of a number of key parameters. Subject to the known limitations of inviscid vortex models, our findings indicate that, in principle, it may be possible to stabilize shear layers for relatively large initial perturbations, provided the actuation has sufficiently many degrees of freedom.

S13.03 | Flow control

Date: February 20, 2019

14:00-16:00

Room: SR 07

Parameter study of turbulent drag reduction by spanwise traveling transversal surface waves

Marian Albers (*RWTH Aachen University, Germany*)

14:00

Pascal S. Meysonnat (*RWTH Aachen University, Germany*)

Daniel Fernex (*Technische Universität Braunschweig, Germany*)

Richard Semaan (*Technische Universität Braunschweig, Germany*)

Bernd R. Noack (*LIMSI-CNRS, France, Technische Universität Braunschweig, Germany, Institut für Strömungsmechanik und Technische Akustik (ISTA), Germany, Harbin Institute of Technology, China*)

Wolfgang Schröder (*RWTH Aachen University, Germany, Forschungszentrum Jülich, Germany*)

Friction drag and therefore energy consumption of large passenger aircraft and high-speed trains are strongly determined by turbulent boundary layers. Therefore, there is considerable scientific interest in influencing the turbulent flow field around such slender bodies to decrease the viscous drag. Active techniques, i.e., techniques where external energy is introduced into the system, have shown promising results for turbulent wall-bounded flows. For instance, Jung et al.[1] achieved drag reduction by applying high-frequency spanwise oscillations of the wall, an extensive overview of different active drag reduction methods is given in [2]. In this work, a numerical parameter study of spanwise traveling transversal surface waves [3] in zero-pressure gradient turbulent boundary layer flow is conducted to find optimal control parameters. A total of 84 high-resolution large-eddy simulations (LES) of the actuated turbulent boundary layer with momentum thickness Reynolds number $Re_{\Theta} = 1,000$ are computed, where the amplitude, wave speed, and wavelength are varied in a wide parameter range. The results show drag reduction of up to 26 percent for a setup with long wavelength and high amplitude and a drag increase of up to 27 percent for very short wavelengths. The turbulent flow field of the drag reduced cases is characterized by a strong decrease of the wall-normal vorticity fluctuations and suppressed quasi-streamwise vortices

above the wave surface. A detailed analysis of the results to develop a control system will be presented at the conference.

References

- [1] W. J. Jung, N. Mangiavacchi, R. Akhavan, Suppression of turbulence in wall-bounded flows by high-frequency spanwise oscillations, *Phys. Fluids A* 4(8), 1605-1607 (1992)
- [2] M. Quadrio, Drag reduction in turbulent boundary layers by in-plane wall-motion, *Philos. Trans. R. Soc. London, Ser. A* 369(1940), 1428-1442 (2011)
- [3] S. R. Koh, P. Meysonnat, M. Meinke, W. Schröder, Drag reduction via spanwise transversal surface waves at high Reynolds numbers, *Flow Turbul. Combust.* 95(1), 169-190 (2015)

Cluster-based network model for drag reduction mechanisms of an actuated turbulent boundary layer

Daniel Fernex (*Technische Universität Braunschweig, Germany*) 14:20

Richard Semaan (*Technische Universität Braunschweig, Germany*)

Marian Albers (*RWTH Aachen University, Germany*)

Pascal S. Meysonnat (*RWTH Aachen University, Germany*)

Wolfgang Schröder (*RWTH Aachen University, Germany, Forschungszentrum Jülich, Germany*)

Rishabh Ishar (*Massachusetts Institute of Technology, USA*)

Eurika Kaiser (*University of Washington, USA*)

Bernd R. Noack (*LIMSI-CNRS, France, Technische Universität Braunschweig, Germany, Technische Universität Berlin, Germany, Harbin Institute of Technology, China*)

We present a cluster-based network model describing the coherent structure dynamics under different control laws. Starting point are time-resolved, statistically representative flow snapshots for various control laws. First, these snapshots are clustered into centroids. Then, a deterministic-stochastic model is identified describing the transition on a dynamic network connecting these centroids. The cluster-based network model reveals actuation mechanisms leading to desirable and undesirable performance. This methodology is applied to a LES drag reduction study of wall-turbulence by the authors. Here, the drag of turbulent boundary layer at $Ma = 0.1$ and $Re = 1000$ is reduced by over 20% using wall-normal surface waves in spanwise direction. A large range of wavenumbers, periods and amplitudes is numerically explored and investigated in a single model.

Drag reduction of transversal surface waves for swept flat plates

Pascal S. Meysonnat (*RWTH Aachen University, Germany*) 14:40

Marian Albers (*RWTH Aachen University, Germany*)

Wolfgang Schröder (*RWTH Aachen University, Germany, Forschungszentrum Jülich, Germany*)

Friction drag and thus energy consumption of slender bodies moving with the fluid, e.g., large passenger aircraft, are strongly determined by turbulent boundary layers. Approximately 50% of the friction drag can be attributed to the shear stress distribution over the wetted surface which in turn is a result of the near wall turbulence. Therefore, there is considerable scientific interest in influencing the turbulent flow field around such slender bodies to decrease the viscous drag. Research nowadays focuses on active methods, i.e., the introduction of spanwise velocities into the near-wall flow field, to reduce skin friction. For instance, Jung et al. [1] achieved drag reduction by applying high-frequency spanwise oscillations of the wall, an extensive overview of different active drag reduction methods is given in [2]. Another approach that has been numerically and

experimentally investigated thoroughly in the past are transversal traveling surface waves [4, 3, 5]. In most investigations, the propagation direction is either perfectly perpendicular to the mean flow direction or along the mean flow direction. However, the flow over, e.g., a swept wing is subject to spanwise pressure gradient. Hence, incident angles of the flow against the proposed surface waves have to be taken into account. As a consequence, we consider a turbulent boundary layer flow subject to spanwise traveling transversal surface waves with sweep angles of up to 30 degrees. The results show that a general drag reduction effect persists, however additional effects, e.g., increased pressure drag, have to be accounted for. A detailed analysis of the results will be presented at the conference.

References

- [1] W. J. Jung, N. Mangiavacchi, R. Akhavan, Suppression of turbulence in wall-bounded flows by high-frequency spanwise oscillations, *Phys. Fluids A* 4(8), 1605-1607 (1992)
- [2] M. Quadrio, Drag reduction in turbulent boundary layers by in-plane wall-motion, *Philos. Trans. R. Soc. London, Ser. A* 369(1940), 1428-1442 (2011)
- [3] S. R. Koh, P. Meysonnat, M. Meinke, W. Schröder, Drag reduction via spanwise transversal surface waves at high Reynolds numbers, *Flow Turbul. Combust.* 95(1), 169-190 (2015)
- [4] N. Tomiyama, K. Fukagata, Direct numerical simulation of drag reduction in a turbulent channel flow using spanwise traveling wave-like wall deformation, *Phys. Fluids*, 25, 105115 (2013)
- [5] P. Meysonnat, D. Roggenkamp, W. Li, B. Roidl, W. Schröder, Experimental and numerical investigation of transversal traveling surface waves for drag reduction, *Eur. J. Mech. B-Fluids*, 55, 313-323 (2016)

Turbulent dissipation in drag reduced flows

Bettina Frohnappfel (*Karlsruhe Institute of Technology, Germany*)

15:00

Andrea Cimarelli (*Università Politecnica delle Marche, Italy*)

Yosuke Hasegawa (*The University of Tokyo, Japan*)

Maurizio Quadrio (*Politecnico di Milano, Italy*)

Davide Gatti (*Karlsruhe Institute of Technology, Germany*)

The question whether turbulent dissipation increases or decreases in turbulent channel flows with turbulent skin friction drag reduction is contradictorily discussed in literature. In order to shed light into this issue we choose to investigate it within the Constant Power Input (CPI) framework, in which the total power fed to the system and thus to total energy dissipation rate is given and constant.

We derive new exact relationships between the Reynolds shear stress (i.e. turbulent skin-friction drag) and the dissipation rates of turbulent and mean kinetic energy, along with all terms in the kinetic energy budgets of turbulent channels. An alternative decomposition of the kinetic energy dissipations is adopted, stemming from an extended Reynolds decomposition, in which the mean velocity is additionally split into a laminar component and a deviation from it. A compact representation of the energy fluxes is introduced to understand their relative importance at different values of the Reynolds number. The particular properties of the laminar and deviation component allow deriving exact relationships that link all the energy fluxes with two wall-normal integrals of the Reynolds shear stresses.

The newly-derived relationships show that drag reduction and turbulent dissipation are linked via the two integrals of the Reynolds shear stresses and a power-based Reynolds number only. This implication of this result is discussed for a number of different flow control scenarios which are realized through DNS of turbulent channel flows under CPI.

Turbulent drag reduction by compliant surface tension active wall layer

Alessio Roccon (*TU Wien, Austria., University of Udine, Italy*)

15:20

Francesco Zonta (*TU Wien, Austria.*)

Alfredo Soldati (*TU Wien, Austria., University of Udine, Italy*)

In this work we use Direct Numerical Simulation (DNS) together with a Phase Field Method to study the turbulent Poiseuille flow of two immiscible liquid layers inside a channel. A thin liquid layer (fluid 1) flows on top of a thick liquid layer (fluid 2), such that their thickness ratio is $h_1/h_2 = 0.075$. The two liquid layers have the same density but different viscosities η , specifically we consider the case $\eta_1 < \eta_2$. The problem is described by the shear Reynolds number (Re_τ), by the Weber number (We, which quantifies surface tension effects) and by the viscosity ratio λ (ratio between the viscosity of the two fluids). Compared to a single phase flow at the same shear Reynolds number ($Re_\tau = 300$), in the stratified case we observe an increase of the flow rate of fluid 2 and a strong modification of the turbulence structures near the liquid-liquid interface. Altogether, these observations support the presence of a significant Drag Reduction (DR), whose efficiency depends strongly on the viscosity ratio (λ).

Flexible fibers in turbulent channel flow

Diego Dotto (*University of Udine, Italy*)

15:40

Cristian Marchioli (*University of Udine, Italy*)

In this paper we investigate the dynamics of small flexible fibers in turbulent channel flow. We aim at examining the translational and rotational behavior of fibers with different elongation (parameterized by the aspect ratio) and inertia (parameterized by the Stokes number) with and without fiber-fluid coupling. We use a Eulerian-Lagrangian approach based on direct numerical simulation of turbulence to describe fiber dynamics. Fibers, which are longer than the Kolmogorov length scale, are modelled as chains of sub-Kolmogorov rods connected through ball-and-socket joints that enable bending and twisting. Different mass and volume fractions are considered to investigate two-way coupling effects. Velocity, orientation and concentration statistics, extracted from simulations at shear Reynolds number $Re = 300$ are presented to give insights into the complex fibers-turbulence interactions that arise when non-sphericity and deformability add to fiber inertia. Statistical observables are examined at varying aspect ratio (namely $\lambda_r = b_r/a = 2$ and 5 , with b_r the length of each element r composing the fiber and a its cross-sectional diameter) and varying fiber inertia (considering values of the element's Stokes number, $St_r = 1, 5, 30$). To highlight the effect of flexibility, statistics are compared with those obtained for fibers that translate and rotate as rigid bodies relative to the surrounding fluid. Flexible fibers in the dilute regime appear to undergo the same inertia-driven mechanisms that govern preferential concentration of spherical particles in bounded flows. In such region, bending of flexible fibers with small inertia (resp. large) inertia is enhanced (resp. reduced) by mean shear and turbulent Reynolds stresses. We show that momentum coupling provides an additional bias, which may produce significant quantitative modifications in the statistics of both phases in the semi-dilute regime. In particular, results up to mass fractions of 40% will be presented to show the effect of momentum coupling on fiber preferential concentration and bending.

S13.04 | Flow control

Date: February 20, 2019

16:30-18:30

Room: SR 07

Temporal prediction horizons of adjoint calculations in turbulent flow

Sophie Knechtel (*Technische Universität Berlin, Germany*)

16:30

Jörn Sesterhenn (*Technische Universität Berlin, Germany*)

The adjoint optimization method is widely used in computational fluid dynamics, but challenging in turbulent flow. In each optimization step, in addition to the direct calculation, the adjoint of the linearized Navier-Stokes equations has to be solved. Turbulent flow has unstable fixed points in linear stability theory and the linear solution, as well as the adjoint solution, diverges. Therefore only a short time frame can be considered.

The unstable behaviour can be described in terms of the maximum Lyapunov exponent, whose inverse gives the magnitude of the temporal prediction horizon. It is highly dependant on flow parameters like the Reynolds number, as well as on discretization methods.

In this talk the results of an extensive study on the dependencies of the maximum Lyapunov exponent are presented. The goal is to prolong the temporal prediction horizon, i.e. the time frame, in which the adjoint calculation is feasible. Test cases are the direct numerical simulation of the compressible, two-dimensional turbulent free shear flow and the two-dimensional turbulent boundary layer. Dependencies on the Reynolds number are discussed, as well as on different temporal and spatial discretization methods. The focus will, in particular, be on finite difference discretizations. The use of a suitable formulation of the compressible Navier-Stokes equations and its adjoint counterpart is stressed and several adjoint formulations are presented. In the course of this the difference between the instability behaviour of the “discrete” and “continuous” adjoint formulations are illuminated. The calculations are performed on an efficiently parallelized object-oriented Fortran code.

Adjoint based topology optimization of a duct bend

Stephan Goeke (*Uni Kassel, Germany*)

16:50

Olaf Wunsch (*Uni Kassel, Germany*)

The cooling performance of a duct is a complex interaction between its shape, position inside the surrounding material and the resulting flow. A change in the geometry does hence effect both the pressure loss as well as the temperature distribution. Due to this coupling of heat transfer and fluid flow a numerical solution is often computationally expensive. Lowering the number of these evaluation steps is therefore crucial. A gradient based optimization method promises high optimization speed if the gradient can be computed effortlessly. The adjoint method in particular offers a low computational cost to calculate this gradient and is hence chosen for the optimization.

In this contribution the continuous adjoint equations including conjugate heat transfer are used to optimize a duct bend. A level-set is used to differentiate the fluid and solid regions. The aim of the optimization is to lower the temperature of a wall inside the heated solid domain. The Reynolds number of the initial design is varied and the effects on the optimization are studied. Different approaches to handle the pressure loss are shown.

A numerical RANS-based model of a nanosecond pulsed plasma actuator for flow control over an airfoil

Roozbeh Aslani (*Johannes Kepler University of Linz, Austria*)

17:10

Michael Krieger (*Johannes Kepler University of Linz, Austria*)

Airfoil stall influences the performance of flight vehicles and remains a challenge for the design of modern aircraft. A Dielectric Barrier Discharge (DBD) device seems to be a very promising tool to control the flow over various parts of an aircraft and suppress the separation. A phenomenological model, based on dynamic similarity between experimental setup and numerical simulation, is developed to simulate the control effect of a Nanosecond Dielectric Barrier Discharge (NS-DBD) actuator. A two-dimensional numerical simulation considers the response of the flow past a NACA 0015 airfoil at 14 deg post stall angle of attack and a Reynolds number of 250,000 to pulsed surface heating of the leading edge. The RANS-based numerical results have been obtained for a baseline simulation (no actuation) and an open-loop control simulation of the airfoil. To capture the laminar-turbulent transition a one-equation local correlation-based transition model is implemented. The numerical results of both the baseline and the actuated case are in good agreement with experiments performed by other authors. The generated coherent vortices seem to have the major control authority to suppress the leading edge separation resulting in flow reattachment.

S14 | Applied analysis

Organiser: Ulisse Stefanelli (*University of Vienna, Austria*)
Patrick Dondl (*University of Freiburg, Germany*)

S14.01 | Applied analysis

Date: February 19, 2019
Room: HS 32

08:30-10:30

Mathematical modeling of structure and function in interacting cell systems

Angela Stevens (*University of Münster, Germany*)

08:30

Developmental processes of interacting cellular systems are driven by different types of cell-cell communication. We model and distinguish between direct/local interactions and communication by diffusive and long-range signaling. The resulting systems of PDEs, of non-local operators, and PDE-ODE-systems are analyzed w.r.t. their pattern forming behavior. An interesting question is, which type of pattern can arise due to which type of interaction.

A bulk-surface reaction-diffusion system for cell polarization

Matthias Röger (*Technische Universität Dortmund, Germany*)

09:10

Barbara Niethammer (*Universität Bonn, Germany*)

Juan J. L. Velázquez (*Universität Bonn, Germany*)

We consider the polarization of a cell in response to a signal. The mathematical model consists of a diffusion equation in the inner volume coupled to a reaction diffusion system on the cell membrane. The system depends on an outside stimulus. In a certain asymptotic limit we rigorously prove the convergence towards a generalized obstacle problem. In term of this limit system we derive conditions for the onset of polarization.

A PDE model for bleb formation and interaction with linker proteins

Philipp Werner (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

09:30

Martin Burger (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

Bleb development of cell membranes occurs during biological processes such as apoptosis, cytokinesis, cell spreading, or viral infection. For some cell types, e.g. tumor cells or primordial germ cells, it also seems to be an alternative means for migration, which itself is an important part in organogenesis and homeostasis.

In contrast to other membrane protrusions like lamellipodia, blebbing is triggered by the cytosol pushing out parts of the cell membrane that separated from the cell cortex, i.e., it is mostly pressure-driven. Besides experimental investigations like micropipette experiments, several biophysical and mathematical models have been developed in order to study bleb development theoretically and numerically.

We present a semilinear fourth order parabolic partial differential equation describing the evolution of the cell membrane, which is coupled to densities of proteins linking the cell membrane to the cell cortex. It incorporates models of linker rupture and repair as well as their diffusive

behaviour. Existence of both time-dependent and stationary solutions of the variational formulation is shown by application of Schauder's fixed point theorem. Further analytic investigations assure physically sensible properties of the solutions: The densities of all linker types prove to be non-negative. Moreover, the H2 norm of the membrane height can be bounded by the L2 norm of the pressure; vice versa, if the pressure is high enough, the membrane height cannot lie beneath a certain critical height almost everywhere. Also, certain stationary solutions are locally exponentially stable against mass conserving disturbances. For vanishing diffusivities, we can express stationary solutions as critical points of an energy functional, which we parametrise with a rate of linker rupture. Sending this rate to infinity, we show that our energy functional Gamma-converges to the energy functional of a blebbing model of Lim, Chiam, and Mahadevan.

Balanced viscosity solutions for infinite-dimensional multi-rate systems

Riccarda Rossi (*Universita' degli studi di Brescia, Italy*)

09:50

Alexander Mielke (*WIAS, Berlin & Humboldt Universitat, Berlin*)

Several mechanical systems are modeled by the static momentum balance for the displacement u coupled with a rate-independent flow rule for some internal variable z . We consider a class of abstract systems of PDEs with this structure, and regularize both the static equation and the rate-independent flow rule by adding viscous dissipation terms with coefficients ε^α and ε , where $\alpha > 0$ is a fixed parameter and $\varepsilon \downarrow 0$. Therefore for $\alpha \neq 1$ the variables u and z have different relaxation rates.

We address the vanishing-viscosity analysis as $\varepsilon \downarrow 0$ of the viscous system. We prove that, up to a subsequence, (reparameterized) viscous solutions converge to a parameterized curve yielding a Balanced Viscosity solution to the original rate-independent system, and providing an accurate description of the system behavior at jumps. In particular, we show that the viscosity in u and the one in z are involved in the jump dynamics in different ways, according to whether $\alpha > 1$, $\alpha = 1$, and $\alpha \in (0, 1)$.

On Fokker-Planck equations with mass evolution

Ina Humpert (*Westfälische Wilhelms-Universität Münster, Germany*)

10:10

Jan-Frederik Pietschmann (*Technische Universität Chemnitz, Germany*)

Martin Burger (*Friedrich-Alexander Universität Erlangen-Nürnberg, Germany*)

In this talk, we present recent results on a Fokker-Planck equation where the mass is not preserved in the evolution. This is realised either by in- and outflow boundary conditions or by spatially homogeneous reaction terms. Our motivation is the growth of neurites, i.e. extensions of a neuron that connect to other cells in its surroundings. We are able to prove exponential decay towards the equilibrium solution using entropy methods. As there is no conservation of mass it is difficult to formulate a classical gradient flow structure which renders the analysis more challenging. In particular, we will explain why classical logarithmic Sobolev inequalities are not applicable any more. Finally, we will present extensive numerical studies that illustrate our analytic results.

S14.02 | Applied analysis

Date: February 19, 2019

08:30-10:30

Room: SR 08

A higher order geometrically nonlinear Cosserat-shell model with initial curvature effects

Patrizio Neff (*Universität Duisburg-Essen, Germany*)

08:30

Mircea Birsan (*Universität Duisburg-Essen, Germany*)

Ionel-Dumitrel Ghiba (*Alexandru Ioan Cuza University of Iasi, Romania*)

We consider an isotropic, three-dimensional, geometrically nonlinear Cosserat material model for thin, curved shells in a variational setting. We perform an analytic dimensional reduction by a higher order ansatz for deformations and rotations over the thickness. The resulting variational problem is stated with respect to a virtual flat reference configuration and entirely expressed in Cartesian coordinates.

The effects of the initial curvature are mapped via multiplicative decomposition of the thin shell deformation. Interestingly, we obtain a model up to fifth-order terms in the thickness, provided the initial shell configuration is curved. In the case of an initially flat (plane) shell, these fifth-order terms are absent.

An existence proof for the nonlinear thin shell will be sketched. Possible extensions to elastoplasticity and shells with applied prestress will be outlined.

Idealized pure and simple shear

Jendrik Voss (*University of Duisburg-Essen, Germany*)

09:10

Christian Thiel (*University of Duisburg-Essen, Germany*)

Robert J. Martin (*University of Duisburg-Essen, Germany*)

Patrizio Neff (*University of Duisburg-Essen, Germany*)

We demonstrate that a deformation corresponding to a Cauchy pure shear stress is not a simple shear. In addition, conditions under which Cauchy pure shear stresses correspond to (idealized) pure shear stretch tensors are stated and a new notion of idealized finite simple shear is introduced.

Tikhonov regularization including tolerances in parameter space

Georgia Sfakianaki (*University of Bremen, Germany*)

09:30

Iwona Piotrowska-Kurczewski (*University of Bremen, Germany*)

Peter Maass (*University of Bremen, Germany*)

Tikhonov regularization for the solution of ill-posed inverse problems is well established. A Tikhonov functional consists of a discrepancy and a regularization term. The former measures the distance between the operator evaluation and the observed data while the latter is used for stabilization of the solution. Motivated by applications in the field of production engineering and new material development, we require the regularized solution to lie within a confidence interval, i.e., we allow small deviations in the solution. Moreover, we are interested in obtaining solutions that are sparse with respect to a given orthonormal basis for the parameter space. In order to model small deviations in the solution, we consider a modified Tikhonov functional with a tolerance measure (dependent on a parameter ϵ) introduced in the regularization term. In

this case, however, sparsity is lost and a way to avoid this problem is by adopting an elastic-net regularization approach.

In this talk, we consider an elastic-net functional consisting of a discrepancy term, an (l^2, ϵ) -penalty term for incorporating tolerances, and an l^1 -penalty term for promoting sparsity in the solution. We discuss the well-posedness of minimizers and exploit the optimality condition for minimizers of this functional.

Variational problems involving Caccioppoli partitions

Sven Torndquist (*WIAS im Forschungsverbund Berlin e.V., Germany*)

09:50

This is an overview of a master's thesis finished in 2017 at the university of Hamburg. The existence and regularity of energy minimising partitions of a bounded domain is discussed. The energy functional appears as a surface energy between the chambers of the partition and is allowed to have a dependency on the neighbouring chambers and the shape of the interface between them. This leads to a problem of anisotropic character. Switching to different settings describing the same problem to treat the subproblems respectively, the key tool to discuss the regularity is the so called "Elimination Lemma" from G.P. Leonardi allowing to reduce the partitioning problem to a simpler problem where locally the minimisation of a reduced energy of just one interface is considered. Here the main effort was to translate Leonardi's result into an anisotropic context which was stated in his original paper. As a consequence we conclude the almost everywhere regularity of the interfaces of minimising partitions.

Homogenization and dimension reduction of a textile shell in linear elasticity

Stephan Wackerle (*Fraunhofer ITWM, Germany*)

10:10

Georges Griso (*LJLL, UPMC, France*)

Julia Orlik (*Fraunhofer ITWM, Germany*)

In this work we investigate textiles and derive their macroscopic properties via simultaneous homogenization and dimension reduction. As reference domain we consider a canvas structure, which we assume to consist of periodically oscillating and isotropic beams with periodicity ε and radius r . Furthermore, the beams are in contact and thereby the elasticity problem is restricted on a cone fulfilling non-penetration and gap conditions.

To obtain different compactness results for all components of the displacement, we apply the decomposition of displacements for beams [1], yielding an elementary and a warping displacement. The derived estimates heavily depend on the small parameters, the elastic energy and the contact. Moreover, we introduce an adapted unfolding operator [2] with an incorporated dimension reduction from three to two dimensions. The properties of the unfolding operator together with the compactness results leads to the weak convergence, which is equivalent to the two-scale convergence. Consequently, the unfolded limits of the displacements, the strain tensor and contact condition yield homogenized 2D-model for a textile.

[1] G. Griso. Decomposition of displacements of thin structures. *J. Math. Pures Appl.* 89 (2008), 199-233.

[2] D. Cioranescu, A. Damlamian and G. Griso. The periodic unfolding method in homogenization. *SIAM J. Math. Anal.* 40 (4), 2008, 1585-1620.

S14.03 | Applied analysis

Date: February 19, 2019

16:30-18:30

Room: HS 32

On the long time behavior of a tumor growth model

Elisabetta Rocca (*University of Pavia, Italy*)

16:30

We consider the problem of the long time dynamics for a diffuse interface model for tumor growth. The model describes the growth of a tumor surrounded by host tissues in the presence of a nutrient and consists in a Cahn-Hilliard-type equation for the tumor phase coupled with a reaction-diffusion equation for the nutrient concentration. We prove that, under physically motivated assumptions on parameters and data, the corresponding initial-boundary value problem generates a dissipative dynamical system that admits the global attractor in a proper phase space. This is a joint work with Alain Miranville and Giulio Schimperna.

Analysis of a Cahn-Hilliard-Brinkman model for tumour growth with chemotaxis

Matthias Ebenbeck (*Universität Regensburg, Germany*)

17:10

Harald Garcke (*Universität Regensburg, Germany*)

Phase field models recently gained a lot of interest in the context of tumour growth models. Typically Darcy-type flow models are coupled to Cahn-Hilliard equations. However, often Stokes or Brinkman flows are more appropriate flow models. In this talk, I will introduce and mathematically analyse a new Cahn-Hilliard-Brinkman model for tumour growth allowing for chemotaxis. Outflow boundary conditions are considered in order not to influence tumour growth by artificial boundary conditions. Based on a recent work [1], I will present ideas to show existence of global-in-time weak solutions in a very general setting.

[1] M. Ebenbeck, H. Garcke, Analysis of a Cahn-Hilliard-Brinkman model for tumour growth with chemotaxis, 2018, <https://arxiv.org/pdf/1807.00705.pdf>.

Patterns and waves in nonlocal reaction-diffusion equations

Christian Kuehn (*Technical University of Munich, Germany*)

17:30

Recently, nonlocality has emerged as a highly active theme in differential equations. In my talk, I shall give several examples of PDEs, where nonlocal effects play a, sometimes quite surprising, role. We start with dynamics of the FKPP equation with nonlocal convolution terms, then proceed to waves in the fractional-diffusion Nagumo equation, and then consider nonlocal modulation equations with convolution terms. The results are based upon the following works: Pattern formation in the doubly-nonlocal Fisher-KPP equation, C. Kuehn and P. Tkachov, arXiv:1805.02116, 2018.

Validity of amplitude equations for nonlocal nonlinearities, C. Kuehn and S. Throm, Journal of Mathematical Physics, Vol. 59, 071510, 2018.

Traveling waves for bistable evolution equations with nonlocal-diffusion, F. Achleitner and C. Kuehn, Advances in Differential Equations, Vol. 20, No. 9-10, pp. 887-936, 2015.

Analysis and numerics of travelling waves for asymmetric fractional reaction-diffusion equations, F. Achleitner and C. Kuehn, Communications in Applied and Industrial Mathematics, Vol. 6, No. 2, 2015

On bounded positive stationary solutions for a nonlocal Fisher-KPP equation, F. Achleitner and C. Kuehn, Nonlinear Analysis A: Theory, Methods & Applications, Vol. 112, pp. 15-29, 2015

Volume-surface reaction-diffusion systems arising from cell biology: analysis and numerics

Bao Quoc Tang (*University of Graz, Austria*)

17:50

This talk presents results on volume-surface reaction-diffusion systems arising from asymmetric stem cell division. During asymmetric stem cell division, the asymmetric localisation of certain proteins called cell-fate determinants leads to two different daughter cells. The localisation of those proteins is observed in *Drosophila* SOP cells to obey two significant processes: diffusion (both in the cell cytoplasm and cell membrane) and biochemical reactions. We propose and study volume-surface reaction-diffusion systems capturing the mentioned processes. For the analysis, we emphasise in particular the fast reaction limit, which gives a new derivation of dynamical boundary conditions, and the exponential convergence to equilibrium by entropy method. We also propose a conservative numerical scheme, meaning that the discrete solution preserves physical properties of the continuum model such as mass conservation, dissipation of energy, and exponential convergence to equilibrium.

On a Lotka-Volterra reaction-diffusion-ODE system with the superimposed interaction between two Neolithic populations

Jan Elias (*University of Graz, Austria*)

18:10

Danielle Hilhorst (*CNRS and University Paris 11, France*)

Masayasu Mimura (*Meiji University and Musashino University, Japan*)

Yoshihisa Morita (*Ryukoku University, Japan*)

M. Humayun Kabir (*Jahangirnagar University, Bangladesh*)

Mathematical modelling plays an increasingly important role in ecology and evolution. Effective models with advanced data analysis improve understanding of the natural world by revealing how the dynamics of species (including human) populations are determined by fundamental biological conditions and processes. The Neolithic transition in Europe involving the change from foraging (hunting and gathering) to agriculture is one of such examples. We have recently proposed a reaction-diffusion model which describes the spatio-temporal evolution of sedentary and migrating farmers and hunter-gatherers in the Neolithic transition. Ecologically, the model stems from the fact that a lifestyle of agriculture and settlement, as an evolutionary advantageous trait, can support a much larger population density than hunting and gathering. Therefore, in our modelling framework, we assume that farmers do not migrate unless they are "forced" due to increased population density pressure. In the talk, we consider a singular limit of the model when a small parameter (a switching parameter between the farming populations) tends to zero. As a result, the spread of farmers is modelled by a nonlinear porous medium type diffusion equation.

S14.04 | Applied analysis

Date: February 19, 2019

16:30-18:30

Room: SR 08

ϵ -expansion of constrained hyperbolic PDEs

Christoph Zimmer (*TU Berlin, Germany*)

16:30

Robert Altmann (*Universität Augsburg, Germany*)

Nowadays, automatic modeling software like Simulink or Dymola/OpenModelica is industrial standard. These tools allow to generate realistic models by interconnecting smaller physical submodels. If the submodels are hyperbolic PDEs then the generated model is a hyperbolic PDE with constraints (PDAE), where normally the interconnection causes the constraints. Classical examples of hyperbolic PDAEs can be found in electrical circuits or gas networks.

In this talk we will investigate hyperbolic PDAEs with a slow and a fast moving state. With the help of gas networks, we investigate how one can approximate such systems by a family of parabolic PDAEs. We prove the approximation orders of different variables under mild assumptions and show that they are optimal. Furthermore, we show how the orders improve under more regular data.

Asymptotic analysis of the visco-acoustic equations for absorbing walls of arrays of Helmholtz resonators

Adrien Xavier Semin (*Technische Universität Darmstadt, Germany*)

16:50

Kersten Schmidt (*Technische Universität Darmstadt, Germany*)

We will consider the visco-acoustic equations in a three-dimensional domain that contains a wall constituted of arrays of Helmholtz resonators. These arrays of resonators are used to suppress reflections from walls. Due to the smallness of the periodicity and of the perforations a direct numerical simulation, e.g., with the finite element method (FEM), is only possible for very large costs. We combine a multiscale approach for the homogenization of the array of Helmholtz resonators with a matched asymptotic method around their aperture to prove that the solution of the visco-acoustic problem admits a limit as the characteristic sizes of the periodicity and of the perforation tend to 0. We justify that the limit model takes the array of Helmholtz resonators into account through equivalent impedance boundary conditions, which integrated into numerical methods like the FEM or the boundary element method leads to much lower computational costs. These impedance boundary conditions are an extension of the transmission conditions derived in [1].

[1] K. Schmidt, A. Semin, A. Thöns-Zueva and F. Bake, On impedance conditions for circular multiperforated acoustic liners, arXiv:1801.04147 (2018).

Dimension reduction and homogenization of a linear elastic periodic shell

Michael Hauck (*Fraunhofer ITWM, Germany*)

17:10

Julia Orlik (*Fraunhofer ITWM, Germany*)

In this work we consider a thin shell of thickness δ , which consists of a periodic pattern, small compared to the other length scales in the problem, of size $\theta\delta$, with $\theta \in (0, \infty)$. We assume that the applied forces on the shell are given such that the total elastic energy is of order $\mathcal{O}(\delta^{\frac{3}{2}})$. Furthermore, the shell is obtained by a diffeomorphism on some reference domain.

We first decompose the displacements acting on the shell into the mid-surface displacement and some warping. Thereafter, we apply a rescaling and unfolding operator to decouple the small parameters from the macroscopic ones and obtain estimates on each shell displacement component in terms of small parameters and derive the limit behavior of the strain tensor when δ tends to 0. By plugging in our decomposition into the weak formulation and passing to the weak limit for linear elasticity we obtain the homogenized shell problem. The procedure is similar to the homogenization of a plate, see for example [Griso, 2018] and [Velcic, 2018]. These results can further be used in problems involving the design optimization with respect to some given functional.

Thermodynamically consistent modelling and analysis of bulk-surface systems with sorption and surface chemistry

Björn Augner (*Technische Universität Darmstadt, Germany*)

17:30

Dieter Bothe (*Technische Universität Darmstadt, Germany*)

Bulk-surface systems play a prominent role in heterogeneous catalysis for chemical engineering. In mathematical analysis, semilinear reaction-diffusion systems with a Fickian model up to now are a very active area of mathematical research with still open and challenging problems. On the other hand, it is well-known that except for low concentrations of solutes in a solvent, the Fickian diffusion model is neither thermodynamically consistent nor physically correct, i.e. cross-effects should be taken into account for non-dilute systems. Moreover, most research so far has been concerned with pure bulk models in an open domain Ω and static boundary conditions, e.g. no flow (homogeneous Neumann) b.c. Recently, more and more focus lies on bulk-surface systems where chemical substances may adhere to an active surface Σ and diffuse on the surface. Based on the conservation law for the concentrations c_i of the species A_i in the bulk and c_i of their adsorbed version A_i^\bullet on the surface the molar fluxes j_i and j_i^Σ (e.g. via Maxwell-Stefan relations), the chemical reaction rates r_i and r_i^Σ (e.g. mimicking standard mass-action-kinetics) and the sorption rates s_i^Σ have to be modelled based on realistic models (e.g. Henry, Langmuir or Freundlich model) for the chemical potentials μ_i and μ_i^Σ . For these models to be physically relevant, consistency with thermodynamics has to be ensured: An entropy principle (or an energy principle) needs to be fulfilled, the structure of the constitutive relations has to ensure positive invariance for the concentrations c_i and c_i^Σ , and when considering a maximal capacity c_S^Σ on the surface the vacancy density needs to be positive as well. We then address the problems of well-posedness, positive invariance and global existence for strong and weak solutions.

The quasiconvex envelope of conformally invariant planar energy functions

Robert J. Martin (*Universität Duisburg-Essen, Germany*)

17:50

Jendrik Voss (*Universität Duisburg-Essen, Germany*)

Oliver Sander (*Technische Universität Dresden, Germany*)

Ionel-Dumitrel Ghiba (*Alexandru Ioan Cuza University of Iași, Romania*)

Patrizio Neff (*Universität Duisburg-Essen, Germany*)

We consider conformally invariant energies on the group of 2×2 -matrices with positive determinant, i.e. energies W satisfying $W(aR) = W(aFR) = W(F)$ for all $a > 0$ and all proper rotations R , and provide an explicit formula for the (notoriously difficult to compute) quasiconvex envelope QW of these functions. In nonlinear continuum mechanics, energies of this form are usually referred to as (objective, isotropic and) isochoric, and are often additively coupled with a volumetric energy term of the form $f(\det(F))$. Our results, which are based on the representation of W in terms of the singular values of the deformation gradient F , can directly be applied to a number of well-known energy potentials, demonstrating the convenience of the eigenvalue-based expression, especially when compared to the representation in terms of the so-called distortion function

commonly used in the context of conformal and quasiconformal mappings. This approach also allows us to answer a conjecture connected to so-called Grötzsch problems.

The fractional p-Laplacian emerging from discrete homogenization of the random conductance model with degenerate ergodic weights

Martin Heida (*WIAS Berlin, Germany*)

18:10

Franziska Flegel (*WIAS Berlin, Germany*)

We study a general class of discrete p-Laplace operators in the random conductance model with long-range jumps and ergodic weights. Using a variational formulation of the problem, we show that under the assumption of bounded first moments and a suitable lower moment condition on the weights, the homogenized limit operator is a fractional p-Laplace operator. Under strengthened lower moment conditions, we can apply our insights also to the spectral homogenization of the discrete Laplace operator to the continuous fractional Laplace operator.

S14.05 | Applied analysis

Date: February 20, 2019

08:30-09:30

Room: HS 32

$C^{1/5-\epsilon}$ weak solutions to the two dimensional Monge-Ampère equation

Wentao Cao (*University of Leipzig, Germany*)

08:30

Laszlo Szekelyhidi Jr. (*University of Leipzig, Germany*)

Monge-Ampère equation is a fully nonlinear, second order partial differential equation with application in isometric embedding, optimal transportation and so on. In this paper, a $C^{1/5-\epsilon}$ weak solution to a two dimensional Monge-Ampère equation is constructed through the technique of convex integration. A planar div-curl system is utilized to diagonalized deficit matrix in every iteration stage and then each stage contains only two steps, which is the key strategy to get a weak solution of $C^{1/5-\epsilon}$ regularity.

A degenerate Cahn-Hilliard model as constrained Wasserstein gradient flow

Clement Cances (*Inria, Univ. Lille, CNRS, France*)

08:50

Daniel Matthes (*TU München, Germany*)

Flore Nabet (*CMAP, Polytechnique, France*)

We study a non-local version of the Cahn-Hilliard dynamics that has been proposed in [W. E and P. Palffy-Muhoray, Phys. Rev. E 55, R3844, 1997]. In difference to the local Cahn-Hilliard equation with nonlinear mobility, one only asks that the divergences of the fluxes - but not necessarily the fluxes themselves - of the two components annihilate each other. Our numerical experiments indicate that due to that higher degree of freedom for the velocity fields, the free energy decays faster in the non-local model than in the local one.

Our main result is a rigorous proof of existence of weak solutions to the non-local equation. The starting point is the formal representation of the dynamics as a constrained gradient flow in the Wasserstein metric. We then show that time-discrete approximations by means of the incremental minimizing movement scheme converge to a weak solution in the limit.

Sharp interface limit of a Stokes/Cahn-Hilliard system

Helmut Abels (*University Regensburg, Germany*)

09:10

Andreas Marquardt (*University Regensburg, Germany*)

We consider the sharp interface limit of a coupled Stokes/Cahn-Hilliard system, when a parameter ϵ that is proportional to the thickness of the diffuse interface tends to zero. The analysis is done in a two dimensional bounded domain with suitable boundary conditions. For sufficiently small times we prove convergence of the solutions of the Stokes/Cahn-Hilliard system to solutions of a sharp interface model, where the Stokes system together with the Young-Laplace law for the jump of the stress tensor is coupled to a Mullins-Sekerka equation with additional convection term, which describes the evolution of the interface. To this end we construct a suitable approximation of the solution of the Stokes/Cahn-Hilliard system and estimate the difference with the aid of a suitable refinement of a spectral estimate of the linearized Cahn-Hilliard operator.

S14.06 | Applied analysis

Date: February 20, 2019

14:00-16:00

Room: HS 32

Rate-independent processes with time-discontinuous data

Dorothee Knees (*University Kassel, Germany*)

14:00

Chiara Zanini (*Politecnico di Torino, Italy*)

Rate-independent processes typically exhibit nonsmooth behavior even if the given data are smooth in time. If the underlying energy functional is nonconvex, then discontinuous solutions appear. Meanwhile, there is a wide variety of solution concepts dealing with such discontinuities. However, in these investigations it is typically assumed that the given data (applied loads in the mechanical context) are in some sense differentiable with respect to time. But this excludes processes, where for instance the loads are switched on or off instantaneously. The aim of this lecture is to discuss for a prototypical rate-independent model with a nonconvex energy functional a solution concept that allows for discontinuous data. The idea is to start from a vanishing viscosity procedure and to identify as precisely as possible the limit process. If time permits, fine properties of the solution sets are analyzed. The lecture relies on joint work with Chiara Zanini (Politecnico di Torino) and on discussions with Pavel Krejci.

Convergence of the Allen-Cahn equation to mean curvature flow with 90°-contact angle

Helmut Abels (*University of Regensburg, Germany*)

14:20

Maximilian Moser (*University of Regensburg, Germany*)

We consider the sharp interface limit of the Allen-Cahn equation with homogeneous Neumann boundary condition in 2D, when a diffuse interface has developed and intersects the boundary of the domain. Here a small parameter in the equation, which is related to the thickness of the diffuse interface, is sent to zero. The limit problem is given by mean curvature flow with a 90°-contact angle condition and convergence using strong norms is shown for small times. Based on a curvilinear coordinate system and asymptotic expansions we construct an approximate solution for the Allen-Cahn equation and estimate the error with a spectral estimate for the linearized Allen-Cahn operator. If time allows I could also comment on recent developments (e.g. higher dimension, vector-valued equation).

Effective diffusion in thin structures via generalized gradient systems and EDP-convergence

Thomas Frenzel (*Weierstrass Institute Berlin, Germany*)

14:40

Matthias Liero (*Weierstrass Institute Berlin, Germany*)

In this talk we discuss the notion of Energy-Dissipation-Principle convergence (EDP convergence) to derive effective evolution equations for gradient systems. In particular, we consider the diffusion of a species in a structure consisting of several thin layers, and we are interested in the limit of vanishing layer thickness. We assume that the thicknesses of the sublayers tend to zero with different rates and the diffusion coefficients scale suitably. This setting can be found for example in organic thin-film semiconductor devices. The evolution of the species concentration can be formulated via a gradient-flow equation with respect to the logarithmic relative entropy of the system and a quadratic Wasserstein-type gradient structure. We show the EDP-convergence of the gradient system by proving suitable asymptotic lower limits of the entropy and the total dissipation functional. The crucial point is that the limiting evolution is again described by a gradient system, however, now the dissipation potential is not longer quadratic but is given in terms of the hyperbolic cosine. The latter describes jump processes across the thin layers and is related to the Marcelin-de Donder kinetics.

Rate-independent evolution of sets & application to fracture processes

Marita Thomas (*Weierstrass Institute for Applied Analysis and Stochastics, Germany*)

15:00

Ulisse Stefanelli (*University of Vienna, Austria*)

Riccarda Rossi (*University of Brescia, Italy*)

This contribution deals with the rate-independent evolution of a set Z of finite perimeter. Its evolution is governed by the interplay of a time-dependent forcing term with the perimeter-term and with a rate-independent dissipation metric related to the volume. We give a notion of solution in terms of a stability condition, discuss fine properties of solutions, and study the validity of an energy-dissipation balance. From this abstract set-model we draw links to delamination and fracture problems, where the set Z is related to the crack-set.

Non-uniqueness for the transport equation with Sobolev vector fields

Stefano Modena (*Universität Leipzig, Germany*)

15:20

We construct a large class of examples of non-uniqueness for the linear transport equation and the transport-diffusion equation with divergence-free vector fields belonging to Sobolev spaces. Our result can be seen as a counterpart to DiPerna and Lions' well-posedness theorem (joint with L. Székelyhidi).

Evolution of vector fields on flexible curves and surfaces

Georg Dolzmann (*Universität Regensburg, Germany*)

15:40

Christopher Brand (*Universität Regensburg, Germany*)

The analysis of the evolution of hypersurfaces driven by geometric flows has a long history. In this talk we present first analytical results for models that couple such a geometric flow with the evolution of a vector field which may represent the orientation of lipid molecules in a liquid bilayer which is ubiquitous in cells.

S14.07 | Applied analysis

Date: February 20, 2019

14:00-16:00

Room: SR 08

Wellposedness of a piezoelectric partial differential equation system - analysis and application

Veronika Schulze (*Paderborn University, Germany*)

14:00

Benjamin Jurgelucks (*Paderborn University, Germany*)

Piezoelectric samples as smart materials are increasingly important in industry and research. In order to interpret the results of a numerical simulation, the existence and uniqueness as well as the regularity of the system must be shown in advance.

In this talk we will consider the proof of wellposedness for a linear piezoelectric model with Rayleigh damping given by a 2nd order coupled partial differential equation system. The difficulty of the proof is based on the included Rayleigh damping terms. Inspired by existing work we develop a proof, which uses in the essential step the Gronwall inequality and handle in such a way the additional damping terms. Higher regularity can also be achieved by additional requirements on the initial and boundary values.

Finally, an application of the results for an open-source FEM simulation will be presented.

Some regularity results for a non-isothermal Cahn-Hilliard model

Andrea Zfferi (*WIAS im Forschungsverbund Berlin e. V., Germany*)

14:20

In this talk I will show and discuss some regularity results for a thermodynamically consistent non-isothermal Cahn-Hilliard model on a bidimensional torus. In the literature, the very same problem has been studied in three and two dimensions including the fluid velocity equations: in the three dimensional setting, the notion of solution was very weak and only its global in time existence could be proved. In turn, in the bidimensional framework the existence of a stronger notion of solution could be achieved. In a recent work by M. Eleuteri et al., the solutions are proved to be more regular, making possible to obtain the uniqueness of the solution and then to analyse the asymptotic behaviour of the system. In this work, neglecting the fluid velocity and so letting the nonlinearities being more tractable, we were able to further improve the smoothness of the solution, in particular in the temperature component, implementing a Moser scheme. This then allowed to slender the proof of uniqueness.

Incorrect estimates by the four wave interaction (FWI) system for the Fermi-Pasta-Ulam (FPU) system

Danish Ali Sunny (*University of Stuttgart, Germany, Institute of Space Technology (IST), Pakistan*)

14:40

Sarfraz Farooq (*Institute of Space Technology (IST), Pakistan*)

Valid description of oscillatory wave packets has wide ranging applications in industry and engineering. Modulation or amplitude equations such as N-wave interaction system or the nonlinear Schrödinger equation are used to describe these oscillations in systems that exhibit dispersion. However, these descriptions are not always correct. In fact, there have been counter examples where incorrect estimates have been proved. We formulate the Four wave interaction system as an approximating system for the Fermi-Pasta-Ulam system. For suitable chosen unstable quadratic resonances, we construct incorrect estimates based on the unstable subspaces corresponding to the integer multiple wave numbers. We also show that this phenomenon is not restricted to the chosen wave number but to a continuum.

Controlled oscillations as a sufficient condition for pre-compactness in the space of \mathbb{R} -valued Young measures

Andrija Raguz (*Zagreb School of Economics and Management, Croatia*)

15:00

We formulate a sufficient condition which, we believe, implies a biting variant of the well-known Ball's condition in the statement of the fundamental theorem of \mathbb{R} -valued Young measures. As an illustration of the application of such a result, following the results presented in the paper G. Leoni: A Remark on Compactness for the Cahn-Hilliard Functional, ESAIM COCV 20(2), 517-523 (2014), we formulate a closely related and much simpler conjecture for the formula of Gamma-limit of one-dimensional Cahn-Hilliard functional equipped with non-coercive two-well potential without specifying any type of its behavior at infinity.

A Naghdi type shell model for irregular shells

Matko Ljulj (*University of Zagreb, Croatia*)

15:20

Josip Tambaca (*University of Zagreb, Croatia*)

Zvonimir Tutek (*University of Zagreb, Croatia*)

A shell model is a two-dimensional model of a three-dimensional elastic body which is thin in one direction. There are several linear and nonlinear shell models in the mathematical literature that are rigorously justified starting from the 3d elasticity. Examples in the mathematical literature are membrane shell models, the flexural shell model in linear and nonlinear context and the Koiter shell model in the case of linearized elasticity. Application of a particular model depends on the particular geometry of the shell's middle surface and the boundary condition which allow or disallow inextensional displacements. Furthermore, since the models are usually written in local coordinates high smoothness of geometry is required for the formulation. Therefore, a model applicable for general geometries and boundary conditions is called for.

In this talk a linear and nonlinear Naghdi type shell model will be presented and related to the classical models. These new models are given in terms of a displacement vector and the (infinitesimal) rotation of the cross-section of the shell, both being in H^1 . The models unite different possible behaviors of shells, they are applicable for all geometries and all boundary conditions, no complicated differential geometry is necessary for the analysis of new models and the models are also well formulated for geometries of the middle surface of the shell with corners. The models will be related to classical models and their asymptotic properties (using weak and Gamma convergence) with respect to the small thickness will be presented.

Homogenization of the diffusion equation on plane mesh structures

Matko Ljulj (*University of Zagreb, Croatia*)

15:40

Kersten Schmidt (*Technische Universität Darmstadt, Germany*)

Adrien Xavier Semin (*Technische Universität Darmstadt, Germany*)

Josip Tambaca (*University of Zagreb, Croatia*)

In this paper we use the homogenization theory and a definition of two-scale convergence to elliptic problems defined on domains consisting of curves located in a plane with certain periodic properties. Using this approach we prove that family of solutions of diffusion equations defined on graphs in a plane with repeating periodic unit cells converges to the solution of appropriate diffusion equation defined on the subset of plane, when unit cells size converge to zero.

We additionally show how to perform formal analysis (which in this setting gives the correct limit model) and show several examples of various unit cells appearing in the domain.

S14.08 | Applied analysis

Date: February 20, 2019

16:30-18:30

Room: HS 32

Homogenization of high-contrast Mumford-Shah energies

Caterina Ida Zeppieri (*WWU Muenster, Germany*)

16:30

We prove a homogenization result for Mumford-Shah-type functionals with "degenerate" periodic coefficients. These kind of functionals can be used to model the energy of a brittle periodic material whose constituents have very different mechanical properties. We show that the high-contrast behavior of the constituents leads, in the homogenized limit, to the emergence of interesting macroscopic effects.

Homogenization of linear elasticity with slip-displacement conditions

Tanja Wolfer (*University of Augsburg, Germany*)

16:50

Malte A. Peter (*University of Augsburg, Germany*)

We consider the linearized elasticity problem with slip displacement conditions for a two-scale composite of two solids. Such interface jumps in displacement arise e.g. in contact problems. In order to upscale this problem we assume that one material is connected whereas the other one is disconnected and periodically distributed over the whole domain. The methods of two-scale convergence and periodic unfolding are applied to determine the macroscopic limit problem rigorously.

Homogenization of one-dimensional discrete optimal transport

Peter Gladbach (*Universität Leipzig, Germany*)

17:10

Eva Kopfer (*Universität Bonn, Germany*)

Jan Maas (*Institute of Science and Technology Austria (IST Austria), Austria*)

Lorenzo Portinale (*Institute of Science and Technology Austria (IST Austria), Austria*)

We study the discrete transportation of probability measures on the non-symmetric discretization of the one dimensional interval $[0,1]$ given by the "Wasserstein-like" dynamical formulation introduced by J.Maas in his work "Gradient flows for the entropy for finite markov chains". We are interested in the behaviour of such discrete transportation metrics as the mesh is getting finer. In a very recent work by Gladbach, Kopfer and Maas, the authors proved the Gromov-Hausdorff convergence to the continuous Wasserstein space $(P([0,1]);W_2)$ under additional geometrical assumptions on the mesh, in general dimension. The non symmetric discretization does not satisfy the geometric assumption and represents in fact a counterexample to the convergence to the continuous Wasserstein space. In spite of the convergence of the discrete heat flow to the continuous one, we prove that the Gromov Hausdorff limit is here given by cW_2 where $c < 1$ is a homogenization factor depending on the geometry of the discrete network.

Homogenization result for a solid-solid phase transformations model

Martin Jesenko (*Albert-Ludwigs-Universität Freiburg, Germany*)

17:30

Patrick W. Dondl (*Albert-Ludwigs-Universität Freiburg, Germany*)

In [1], the authors study displacive solid-solid phase transformations. They show that a nearly flat interface is given by the graph of a function u which evolves according to the equation

$$\delta_t u(t, x) = -(-\Delta)^{1/2} u(t, x) + f(x, u(t, x)) + F$$

with f being the local driving force and F an external force. This equation also arises in the study of dislocations and fracture. They show for the periodic setting that such interfaces exhibit a stick-slip behaviour associated with pinning and depinning. Here, we are considering a case where the local driving force is a random function with a very fine distribution given by a small parameter $\epsilon > 0$ and rescale $f_\epsilon(x, y) := f(x/\epsilon, y/\epsilon)$. Let u_ϵ be the solution of

$$\delta_t u(t, x) = -(-\Delta)^{1/2} u(t, x) + f_\epsilon(x, u(t, x)) + F \quad \text{and} \quad u(0, x) = u_0(x).$$

We show that if the initial function u_0 is flat enough, there is a $F^* > 0$ so that for any $F \leq F^*$ the solutions converge to the initial value, i.e. for all $x \in \mathbf{R}^n$ and $t \in \mathbf{R}$

$$\lim_{\epsilon \rightarrow 0} \mathbf{E}[u_\epsilon(t, x) - u_0(x)] = 0$$

To some extent, our result is in correlation with the results in [2] for the periodic deterministic setting.

References

[1] Bhattacharya, K.; Dondl, P. W. Effective behavior of an interface propagating through a periodic elastic medium. *Interfaces Free Bound.* 18 (2016), no. 1, 91-113

[2] Monneau, R.; Patrizi, S. Homogenization of the Peierls-Nabarro model for dislocation dynamics. *Journal of Differential Equations*, 253(7) (2012), 2064-2105

Quantitative stochastic homogenization: recent advances and perspectives

Julian Fischer (*IST Austria, Austria*)

17:50

In recent years, the quantitative stochastic homogenization of partial differential equations has seen tremendous progress, leading in particular to the first proof of optimal homogenization rates for linear elliptic equations by Gloria and Otto and to rates of homogenization for nonlinear equations by Armstrong and Smart. We give an overview of some of the recent results of the author in the field of quantitative homogenization of random media, including higher-order approximation results for linear elliptic PDEs and aspects of numerical algorithms for the computation of effective coefficients.

Transmission, reflection, and refraction at meta-material interfaces

Ben Schweizer (*TU Dortmund, Germany*)

18:10

The Helmholtz equation and the time-harmonic Maxwell equations describe the intensity of waves. In periodic media, interesting phenomena can occur due to resonance effects. Our focus in this talk are interfaces between two media and boundary conditions at infinity, i.e., radiation conditions. We use Bloch expansions to describe both, to analyze negative refraction at interfaces between meta-materials and to construct a stable numerical scheme for radiation conditions in meta-materials.

S14.09 | Applied analysis

Date: February 21, 2019

08:30-10:30

Room: HS 32

Crystallization and discrete differential geometry

Gero Friesecke (*TUM, Germany*)

08:30

Why do atoms typically self-assemble into crystalline order at low temperature? This deep question remains extremely poorly understood from a mathematical standpoint. Closely related, equally poorly understood, problems include:

- sphere packing (recent progress was made in dimensions 24 and 8, but not 3)
- the celebrated Abrikosov vortex lattice in Bose-Einstein condensates
- self-assembly of viruses from their coat proteins.

My goal in this talk is two-fold: (1) to give a general introduction to crystallization problems, (2) to discuss recent progress for a basic model problem, minimization of the Heitmann-Radin energy in 2D. The ground state for any finite number of particles was shown by Heitmann and Radin to be a subset of the triangular lattice, via clever but very technical ad hoc arguments. Recently [1] this result was understood in a novel way via discrete differential geometry, by endowing the bond graph of general particle configurations with the "right" notion of discrete curvature and appealing to a recent discrete Gauss-Bonnet theorem by Knill which relates the sum/integral of curvature to defects and appears to be extremely promising for future work on understanding defects and their cores in crystals in a non-phenomenological way.

[1] L.De Luca, G.Friesecke, Crystallization in two dimensions and a discrete Gauss-Bonnet theorem, *J Nonlinear Sci.* 28, 69-90, 2018

[2] L.De Luca, G.Friesecke, Classification of Particle Numbers with Unique Heitmann-Radin Minimizer, *J. Stat. Phys.* 167, Issue 6, 1586-1592, 2017

A dipolar Gross-Pitaevskii equation with quantum fluctuations: self-bound states

Yongming Luo (*University Kassel, Germany*)

09:10

We prove existence and qualitative properties of standing wave solutions to a generalized nonlocal 3rd-4th order Gross-Pitaevskii equation (GPE), the latter being currently the state-of-the-art model for describing the dynamics of dipolar Bose-Einstein condensates. Using a mountain pass argument on spheres in L^2 and constructing appropriately localized Palais-Smale sequences we are able to prove existence of real positive ground states as saddle points of the energy. The analysis is deployed in the set of possible states, thus overcoming the problem that the energy is unbounded below. We also prove a corresponding nonlocal Pohozaev identity with no rest term, a crucial part of the analysis.

Crystallization in the hexagonal lattice for ionic dimers

Manuel Friedrich (*WWU Münster, Germany*)

09:30

Leonard Kreutz (*WWU Münster, Germany*)

We consider finite discrete systems consisting of two different atomic types and investigate ground-state configurations for configurational energies featuring two-body short-ranged particle interactions. The atomic potentials favor some reference distance between different atomic types

and include repulsive terms for atoms of the same type, which are typical assumptions in models for ionic dimers. Our goal is to show a two-dimensional crystallization result. More precisely, we give conditions in order to prove that energy minimizers are connected subsets of the hexagonal lattice where the two atomic types are alternately arranged in the crystal lattice. We also provide explicit formulas for the ground-state energy. Finally, we characterize the net charge, i.e., the difference of the number of the two atomic types.

Coupled self-organized hydrodynamics and Stokes models for suspensions of active particles

Pierre Degond (*Imperial College London, UK*)

09:50

Sara Merino-Aceituno (*University of Vienna, Austria*)

Fabien Vergnet Vergnet (*Université Paris Sud, France*)

Hui Yu (*Tsinghua University, China*)

We derive macroscopic dynamics for collective motion in a fluid. The starting point is a coupled Vicsek-Stokes system. The Vicsek model describes self-propelled agents interacting through alignment. It provides a phenomenological description of steric interactions between agents at high density. Stokes equations describe a low Reynolds number fluid.

Continuum limit and homogenization of stochastic and periodic discrete systems - fracture in composite materials

Laura Lauerbach (*University of Wuerzburg, Germany*)

10:10

Stefan Neukamm (*TU Dresden, Germany*)

Mathias Schäffner (*University of Leipzig, Germany*)

Anja Schlömerkemper (*University of Wuerzburg, Germany*)

The limiting behaviour of a one-dimensional discrete system is studied by means of Γ -convergence. We consider a toy model of a chain of atoms. The interaction potentials are of Lennard-Jones type. Additionally, we consider them to be periodically or stochastically distributed. The energy of the system is considered in the discrete to continuum limit, i.e. as the number of atoms tends to infinity. During that limit, a homogenization process takes place. The limiting functional will be discussed, especially with regard to fracture. That will lead to a different approach by a rescaled version of the problem. This second ansatz results in a limiting energy of Griffith's type consisting of a quadratic integral term and a jump contribution. The periodic case can be found in [1].

[1] Lauerbach, L. , Schäffner, M. and Schlömerkemper, A. (2018), On continuum limits of heterogeneous discrete systems modelling cracks in composite materials. *GAMM-Mitteilungen*, 40: 184-206. doi:10.1002/gamm.201730003

S14.10 | Applied analysis

Date: February 21, 2019

14:00-16:00

Room: HS 32

Effective theories for atomistically thin films

Bernd Schmidt (*Universitaet Augsburg, Germany*)

14:00

We report on recent results on the derivation of effective continuum theories from atomistic models for thin structures. Special attention is paid to effective properties which are particular to atomistically thin films consisting of only a few atomic layers.

Variance reduction for effective energies of random lattices in the Thomas-Fermi-von Weizsäcker model

Julian Fischer (*IST Austria, Austria*)

14:40

Michael Kniely (*IST Austria, Austria*)

We discuss the calculation of effective energies of random materials described by the Thomas-Fermi-von Weizsäcker (TFW) equations in the framework of the method of representative volume elements (RVEs). The TFW-equations form a coupled system of nonlinear elliptic equations and describe the distribution of electrons in the presence of a prescribed nuclear charge density. The RVE-approximation is subject to a systematic error (due to the restriction to finite material samples) and a random error (due to material differences in different RVEs). Our focus lies on the reduction of the variance of the energy when evaluated for the RVE, as the systematic error decreases exponentially as a function of the diameter of the RVE. This variance reduction can be achieved by choosing the RVE in such a way that it represents the statistical properties of the underlying material particularly well, an approach invented by Le Bris, Legoll, and Minvielle in the numerical homogenization of linear elliptic equations. A rigorous analysis of this strategy has been provided recently by the first author for linear elliptic PDEs.

For proving the variance reduction in the case of the nonlinear TFW-equations, we need a locality result which ensures that perturbations of the nuclear density inside a bounded region result in a change of the electronic density decaying exponentially away from this region. We establish the required locality by extending a recent result by Nazar and Ortner for smeared nuclear charges to the case of point nuclei represented by Dirac measures.

Rigorous derivation of the effective equation of a linear reaction system with different time scales

Artur Stephan (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany, Humboldt-Universität zu Berlin, Germany*)

15:00

Alexander Mielke (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany, Humboldt-Universität zu Berlin, Germany*)

We consider a linear reaction system with slow and fast reactions, and investigate its behavior if some reaction rates tend to infinity. Assuming detailed balance, it is well known that the reaction system can be written as a gradient flow. Focusing on the physical relevant gradient structure which has its motivation from the Theory of Large deviation, we show how an effective limiting equation can be derived rigorously in the sense that the underlying gradient structure is preserved. The limiting process contains only slow reactions coarse-grained with respect to the local equilibria of the fast reactions.

On a Gamma-limit of Willmore functionals with additional curvature penalization term

Heiner Olbermann (*UCLouvain, Belgium*)

15:20

We consider the Willmore functional on graphs, with an additional penalization of the area where the curvature is non-zero. Interpreting the penalization parameter as a Lagrange multiplier, this corresponds to the Willmore functional with a constraint on the area where the graph is flat. Sending the penalization parameter to infinity and rescaling suitably, we derive the limit functional in the sense of Gamma-convergence.

On Kolmogorov's two-equation model for turbulence

Alexander Mielke (*WIAS and HU Berlin, Germany*)

15:40

Kolmogorov's model for turbulence consists of the incompressible Navier-Stokes equations for the velocity field u and the pressure coupled to two scalar parabolic equations for the average frequency ω and the mean turbulent kinetic energy k . The point is that the viscosities in all three equations are proportional to k/ω , which makes the equations quasilinear. Moreover, the dissipative losses of the velocity field u are feeded as source term into the mean kinetic turbulent energy.

We report on joint work [1,2] with Joachim Naumann, where a global existence result for weak solutions with defect measure are derived under the assumption that the initial condition for k is bounded from below by a positive constant. We also discuss the question of existence of similarity solutions.

[1] A. Mielke, J. Naumann: Global-in-time existence of weak solutions to Kolmogorov's two-equation model of turbulence. C.R. Acad. Sci. Paris Ser. I, 353, 321-326, 2015.

[2] A. Mielke, J. Naumann: On the existence of global-in-time weak solutions and scaling laws for Kolmogorov's two-equation model of turbulence. WIAS preprint 2545, 2018, arXiv:1801.02039.

S14.11 | Applied analysis

Date: February 22, 2019

08:30-10:30

Room: HS 32

Dynamic perfect plasticity and damage in viscoelastic solids

Elisa Davoli (*University of Vienna, Austria*)

08:30

Ulisse Stefanelli (*University of Vienna, Austria*)

Tomáš Roubíček (*Charles University, Prague, Czech Republic*)

In this talk we will analyze a system of PDEs and differential inclusions describing the combination of linearized perfect plasticity and damage effects in a dynamic setting for viscoelastic media. In particular, we will show existence of a suitable notion of weak solutions to the constitutive and balance equations of the model.

Coupled advection-reaction-diffusion processes on an evolving microstructure: analysis and homogenization

David Matthias Wiedemann (*University of Augsburg, Germany*)

08:50

Malte A. Peter (*University of Augsburg, Germany*)

We consider a porous medium composed of solid matrix and pore space, which is completely saturated with a fluid. A dissolved concentration is present in the fluid, which is affected by diffusion and advection as well as reaction at the surface of the solid matrix. This reaction causes the solid matrix to grow or shrink locally. Thus, the microstructure of the porous medium changes, which affects the transport of the concentration.

In order to upscale this problem, we consider an advection-reaction-diffusion problem coupled with the Stokes equation in a domain with an evolving microstructure. The homogenization of this problem is performed utilising a transformation to a periodic reference domain and the macroscopic limit problem is determined using two-scale convergence.

A unified model for stress-driven rearrangement instabilities

Paolo Piovano (*University of Vienna, Austria*)

09:10

Morphological destabilizations of crystalline interfaces are often referred to as Stress-Driven Rearrangement Instabilities (SDRI) and Asaro-Grinfeld-Tiller (AGT) instabilities. They consist in various mechanisms of mass rearrangements that take place at crystalline boundaries because of the strong stresses originated by the mismatch between the parameters of adjacent crystalline lattices.

Atoms move from their crystalline order and different modes of stress relief may co-occur, such as deformations of the bulk materials with storage of elastic energy and boundary instabilities penalized by the surface energy.

In this talk we introduce a variational model displaying both elastic and surface energy that simultaneously takes into account the various possible SDRI, such as boundary discontinuities, internal cracks, external filaments, and fractures, and that provides a unified treatment for epitaxially-strained thin films, crystal cavities, grain boundaries, as well as fractures.

More precisely, under a constraint on the maximum number m of boundary components, we prove the existence of minimizing configurations by assessing the compactness of energy-equibounded sequences and the lower semicontinuity of the energy with respect to a suitable topology. Furthermore, as $m \rightarrow \infty$ such minimizing configurations represent a minimizing sequence for the unconstrained model. In particular, we extend previous literature results that were separately obtained in the different settings of thin films and material voids for graph-like boundaries. Joint collaborations with Sh. Kholmatov (Vienna).

Drift-diffusion problems with Gauss-Fermi statistics and field-dependent mobility for organic semiconductor devices

Annegret Glitzky (*Weierstrass Institute Berlin, Germany*)

09:30

We introduce a drift-diffusion model for organic semiconductor devices including Gauss-Fermi statistics and application-specific mobility functions. The charge transport in organic materials is realized by hopping of carriers between adjacent energetic sites and is described by mobility laws with a strong nonlinear dependence on temperature, carrier densities and the electric field strength. First, we summarize analytical results for the stationary problem. Then, the existence of global weak solutions of the stationary problem is proven by considering a problem with (for small densities) regularized state equations on any arbitrarily chosen finite time interval. We ensure its solvability by time discretization and passage to the time-continuous limit. Positive lower a priori estimates for the densities of its solutions that are independent of the regularization level ensure the existence of solutions to the original problem. Furthermore, we derive for these solutions global positive lower and upper bounds strictly below the density of transport states for the densities. The estimates rely on Moser iteration techniques.

Weak-strong uniqueness for Navier-Stokes two-phase flow with surface tension

Sebastian Hensel (*Institute of Science and Technology Austria, Austria*)

09:50

Julian Fischer (*Institute of Science and Technology Austria, Austria*)

We establish a weak-strong uniqueness principle for the flow of two immiscible, incompressible and viscous fluids with surface tension. As long as there exists a strong solution to the system, every varifold solution originating from the same initial condition has to coincide with it. Our result covers the regime of phase-dependent densities and shear viscosities and holds true in two and three spatial dimensions. The global-in-time existence of varifold solutions was established by H. Abels (*Interfaces Free Bound.* 9, 2007). The key ingredient of our result is the construction of a relative entropy functional which is capable of controlling the interface error.

Two-speed solutions to non-convex rate-independent systems

Sebastian Schwarzacher (*University of Prague, Czech Republic*)

10:10

Filip Rindler (*University of Warwick, UK*)

Endre Suli (*University of Oxford, UK*)

Juan J. L. Velázquez (*University of Bonn, Germany*)

Rate-independent systems are time-dependent PDEs, where the time derivative only occurs inside a positively zero-homogeneous dissipational force term. As such, these systems can be thought of as about 'half-way' between elliptic and parabolic systems. In particular, the evolution is quasi-static and jumps may occur in time if the elastic potential is non-convex. If one sees these processes as rescaling limits of parabolic equations, then it becomes clear that the jump evolution may be complicated and in fact needs to be carefully analyzed in order to prove well-posedness and the physically relevant energy dissipation balance. While there are several approaches to the analysis of rate-independent systems, so far questions of regularity, which are intimately tied to the development of a satisfactory solution theory, have not been considered in great detail. In this talk I will present some very recent results on existence, uniqueness, regularity, and approximation for rate-independent systems. Further, I will introduce what we call two-speed solutions which allow to characterize the jump transients in an infinitesimal time variable.

S15 | Uncertainty quantification

Organiser: Hanno Gottschalk (*University of Wuppertal, Germany*)
Claudia Schillings (*University of Mannheim, Germany*)

S15.01 | Uncertainty quantification

Date: February 19, 2019
Room: HS 07

08:30-10:30

Uncertainty quantification with stochastic discontinuities

Andrea Barth (*University of Stuttgart, Germany*)

08:30

Many phenomena in the Sciences and Engineering are modelled by dynamical systems with discontinuous parameters. If, moreover, the parameters are uncertain, a discontinuous random field or stochastic process should be used. The reduced regularity and the involved structure of these random fields lead to a more involved analysis, approximation and simulation of the stochastic dynamical system. When sampling-based methods are used to approximate statistical properties of the solution, the spacial (and/or temporal) discretization has to be adapted to the discontinuities, leading to a sample-adapted discretization. In this talk, I will give an introduction to the modelling of discontinuous random fields. For the approximation of moments of an elliptic problems with jump-diffusion coefficients, a sample-adapted multilevel Monte Carlo method is used. Multilevel Monte Carlo methods were introduced to decrease the computational complexity of the calculation of, for instance, the expectation of a random quantity. More precisely, in comparison to standard Monte Carlo methods, the computational complexity is (asymptotically) equal to the calculation of one sample of the problem on the finest discretization grid used. The price to pay for this increase in efficiency is that the problem must be solved not only on one (fine) grid, but on a hierarchy of discretizations. This implies, first, that the solution has to be represented on all grids and, second, that the variance of the detail (the difference of approximate solutions on two consecutive grids) converges with the refinement of the grid. For discontinuous problems, the multilevel Monte Carlo approach has to be altered accordingly.

Random elliptic PDEs with levy coefficients

Oliver Gerhard Ernst (*TU Chemnitz, Germany*)

09:10

Toni Kowalewitz (*TU Chemnitz, Germany*)

Hanno Gottschalk (*Bergische Universität Wuppertal, Germany*)

Marco Reese (*Bergische Universität Wuppertal, Germany*)

We consider stationary diffusion equations where the diffusion coefficient is a generalized random field with Lévy distribution. We describe the functional analytic setting for such generalized random fields and show how a smoothing procedure yields random PDEs amenable to numerical approximation. Numerical illustrations are provided for 1D and 2D examples.

The diffusion equation with random diffusion coefficient given by (transformed) Lévy fields

Hanno Gottschalk (*University of Wuppertal, Germany*)

09:30

Marco Reese (*University of Wuppertal, Germany*)

Oliver Gerhard Ernst (*TU Chemnitz, Germany*)

Toni Kowalewitz (*TU Chemnitz, Germany*)

We consider diffusion equations with transformed smoothed Lévy noise fields as random diffusion coefficients. We investigate the unique weak solution to this elliptic PDE wrt its integrability and approximability by estimating the extreme values of these fields. With this approach, we can show that solutions possess moments of all order of the Sobolev norm.

We approximate random diffusion coefficient by applying Mercer's theorem on the smoothing kernel of the smoothed Lévy noise field. This approximation provides us the convergence of the appropriate weak solution in the n-th mean to the real weak solution.

Fast simulation of non-stationary Gaussian random fields: the sinc-multilevel approach

Lukas Herrmann (*ETH Zürich, Switzerland*)

09:50

Kristin Kirchner (*ETH Zürich, Switzerland*)

Christoph Schwab (*ETH Zürich, Switzerland*)

We propose a new algorithm for generating samples of Gaussian random fields, whose covariance operators are negative fractional powers of elliptic second-order differential operators. This class of random fields includes the Whittle-Matérn fields which were introduced in [F. Lindgren, H. Rue, and J. Lindström: An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach (with discussion), *J. Roy. Statist. Soc. Ser. B Stat. Methodol.*, 73 (2011), pp. 423-498]. In [D. Bolin, K. Kirchner, and M. Kovács: Numerical solution of fractional elliptic stochastic PDEs with spatial white noise, arXiv:1705.06565] the numerical approximation of such random fields based on a finite element discretization in space and a sinc quadrature for the Balakrishnan integral representation of the negative fractional-order covariance operator has been proposed.

We extend this approach by combining it with various multilevel strategies. Under minimal assumptions on the second-order differential operator determining the covariance structure of the field, we prove that our algorithm generates one sample of the Gaussian random field on an unstructured simplicial triangulation of a bounded Euclidean domain in $d=1,2,3$ dimensions at a total cost with respect to work and memory which is essentially linear in the number of nodes in the triangulation. A key feature of our approach is its applicability to simulating Gaussian random fields whose covariance functions are neither stationary nor asymptotically smooth nor explicitly known.

Applications to multilevel quasi-Monte Carlo finite element methods for PDEs with random coefficients in uncertainty quantification are presented.

Sparse compression of expected solution operators

Daniel Peterseim (*Universität Augsburg, Germany*)

10:10

Michael Feischl (*Universität Bonn, Germany*)

We show that the expected solution operator of prototypical linear elliptic partial differential operators with random coefficients is well approximated by a computable sparse matrix. This result is based on a random localized orthogonal multiresolution decomposition of the solution space that allows both the sparse approximate inversion of the random operator represented in this basis as well as its stochastic averaging. The approximate expected solution operator can be interpreted in terms of classical Haar wavelets. When combined with a suitable sampling approach for the expectation, this construction leads to an efficient method for computing a sparse representation of the expected solution operator.

Reference: <https://arxiv.org/abs/1807.01741>

S15.02 | Uncertainty quantification

Date: February 19, 2019

16:30-18:30

Room: HS 16

Adaptive sparse polynomial chaos expansions: a survey

Nora Lüthen (*ETH Zurich, Switzerland*)

16:30

Bruno Sudret (*ETH Zurich, Switzerland*)

Polynomial Chaos Expansions (PCEs) are a popular surrogate modelling technique that, for a computational model with random input variables, aims to find a spectral representation of the model response in terms of orthogonal polynomial functions of the input variables. We consider non-intrusive regression-based PCEs applicable to black-box models. The coefficients of a PCE can be computed by least-squares regression; however, this needs many model evaluations and is infeasible for high input dimension and high polynomial degree. In contrast, a sparse representation, i.e., one for which only few coefficients are nonzero, can be computed accurately from much fewer model evaluations even for high dimension and high degree.

The process of computing a sparse PCE is modular and consists of the repeated execution of the following components: choice/augmentation of the polynomial candidate set, choice/augmentation of the experimental design, computation of the sparse solution for the current candidate set and experimental design, and evaluation of performance and stopping criteria. For each of these components, a variety of promising methods has been proposed in the literature within the last few years; however, little has been done in terms of comparing the methods available for each component and identifying the optimal combination of methods for the modular procedure.

In this contribution, we present a literature survey for adaptive sparse PCEs together with numerical benchmarking. We give an overview of the available methods, present results of the benchmarking and identify the best combination of methods for the computation of sparse PCE surrogates with high input dimension and/or high polynomial degree.

An intrusive PCE extension of the Contour Integral Method and its application in electrical engineering

Eduard Frick (*Hamburg University of Technology, Germany*)

16:50

David Dahl (*Hamburg University of Technology, Germany*)

Christian Seifert (*Hamburg University of Technology, Germany*)

Marko Lindner (*Hamburg University of Technology, Germany*)

Christian Schuster (*Hamburg University of Technology, Germany*)

The Contour Integral Method (CIM) is an efficient technique for electromagnetic simulations in a parallel plate environment. Such an environment consists of a thin homogeneous dielectric layer that is bounded from the top and the bottom by two perfectly conducting parallel plates. These plates are often connected by several cylindrical conducting vias which act as scatterers of waves. The electric and magnetic fields at a fixed frequency inside the parallel plate environment can be obtained from the solution of a Helmholtz equation, provided that certain additional assumptions are met. This solution is obtained from an equivalent two dimensional boundary integral equation, where the boundary of an infinite plate is defined by the via contours. The deterministic diskretization of the boundary integral equation is transformed into a matrix equation that provides a linear relation between the current and the voltage on the boundary, where the corresponding matrix is called the (parallel plate) impedance matrix and is often the main quantity of interest in the CIM method.

The impedance matrix depends on several configuration parameters and it is then of great importance to be able to model the uncertainty propagation from these parameters to the impedance matrix. This requires the choice of an appropriate numerical method for stochastic simulations. The well-known Monte Carlo (MC) method is easy to implement and reliable but it suffers from slow convergence. One possible alternative to MC, that is often much faster, is the polynomial chaos expansion (PCE). A distinction is made between the so-called intrusive and non-intrusive versions of the PCE. Both are Galerkin projection methods. In the non-intrusive PCE the projection to a finite-dimensional space spanned by orthogonal polynomials in the random variables is applied to the deterministic impedance matrix. In the intrusive PCE the projection is applied to the discretized CIM equation prior to the computation of the impedance matrix. This leads to a stochastic matrix equation that provides a linear relation between the PCE expansion of the current and the PCE expansion of the voltage on the boundary. The focus of this report lies on the intrusive formulation of the CIM method. We explain its implementation and discuss its advantages and disadvantages compared to the non-intrusive PCE and to MC. All three methods are applied to CIM with a varying number of random input parameters and varying input distributions.

Formulation of a spectral stochastic finite element for problems with uncertain geometry

Daniel Trauner (*Technische Universität Wien, Austria*)

17:10

Christian Bucher (*Technische Universität Wien, Austria*)

As an extension of the Finite Element Method (FEM), the Spectral Stochastic Finite Element Method (SSFEM) is widely considered an efficient tool to determine the response of mechanical systems subject to uncertain material properties. The present paper aims to apply the SSFEM to problems with uncertain geometry, in which the system boundary is described via a random field. This leads to Finite Elements with uncertain nodal coordinates, which can be expressed in terms of independent and identically distributed gaussian random variables, by applying the Karhunen-Loeve Expansion on the random field. The system's unknown random field solution is discretized, using the Polynomial Chaos Expansion (PCE), as a function of known random variables and incorporated into the formulation of the finite elements. This results in additional degrees of freedom in each node of these finite elements, corresponding to the number of basis polynomials of the PCE. Applying a Galerkin error minimization approach on the element level and assembling the global stochastic stiffness matrix leads to a deterministic linear system of equations for deterministic coefficients, which ultimately characterize the response.

As an application of this method, the solution of a 2D elasticity problem using Spectral Stochastic CST elements is computed. The resulting response function is subsequently used in a Shape Optimization. The optimization process is computationally cheap, as the response is given as a function of input variables and no further systems of equations need to be solved.

Possible future applications include the analysis of structures sensitive to imperfections resulting in a random eigenvalue problem, and random interface problems.

Model order reduction for linear stochastic Galerkin systems with moments as outputs

Roland Pulch (*Universität Greifswald, Germany*)

17:30

Akil Narayan (*University of Utah, United States*)

We consider linear dynamical systems consisting of ordinary differential equations (ODEs), where a quantity of interest (QoI) is defined as output. In an uncertainty quantification, physical parameters are replaced by random variables. We expand the state variables as well as the QoI

into a series with orthogonal basis polynomials following the concept of the so-called polynomial chaos. The stochastic Galerkin approach yields a larger coupled linear system of ODEs, whose solution represents an approximation of the unknown coefficient functions. Our aim is to obtain the first two statistical moments of the QoI, i.e., the expected value and the variance. In the stochastic Galerkin system, the expected value becomes a linear output, whereas the variance is defined as a quadratic output. Since the stochastic Galerkin system is high-dimensional, we apply model order reduction (MOR) to obtain a low-dimensional system, which still approximates the moments sufficiently accurate. On the one hand, the system of ODEs with a quadratic output is equivalent to a system with a large number of linear outputs. On the other hand, an equivalent quadratic-bilinear system exists with just two linear outputs. We investigate the quadratic-bilinear approach further, where specific MOR methods are applied. Results of numerical computations are presented for a test example.

A higher order perturbation approach for electromagnetic scattering problems on random domains

Jürgen Dölz (*TU Darmstadt, Germany*)

17:50

We are interested in time-harmonic electromagnetic scattering problems on scatterers with uncertain shape. Thus, the scattered field will also be uncertain. Based on the knowledge of the two-point correlation of the domain boundary variations around a reference domain, we derive a perturbation analysis of the mean of the scattered field. The approach is based on the second shape derivative of the scattering problem and will be at least third order accurate in the perturbation amplitude of the domain variations. To compute the required second order correction term, a tensor product equation on the domain boundary has to be solved. We discuss its discretization and efficient solution using boundary integral equations. Numerical experiments in three dimensions will be presented.

Padé-based model order reduction for parametric/stochastic Helmholtz frequency response problems

Francesca Bonizzoni (*University of Vienna, Austria*)

18:10

Fabio Nobile (*Ecole Polytechnique Fédérale de Lausanne, Switzerland*)

Ilaria Perugia (*University of Vienna, Austria*)

Davide Pradovera (*Ecole Polytechnique Fédérale de Lausanne, Switzerland*)

This talk deals with the parametric/stochastic time-harmonic wave equation, where the (random) parameter is the wavenumber, sweeping a given interval of interest. We introduce the Helmholtz frequency response function, that is, the map which associates to each wavenumber the solution of the corresponding Helmholtz problem endowed with mixed Dirichlet/Neumann boundary conditions. We are interested in knowing the Helmholtz frequency response function for all the (random) parameter values ranging in the given interval of interest.

Due to the oscillatory behavior of the solutions, the finite element approximation of Helmholtz frequency response problems in mid- and high-frequency regimes is challenging: accurate approximations are possible only on very fine meshes or with high polynomial approximation degrees. For this reason, the direct numerical evaluation of the Helmholtz frequency response function for a whole range of frequencies is out of reach.

When extended to the complex plane (i.e., considering complex wavenumbers), the Helmholtz frequency response function is proved to be meromorphic, with a pole of order one in every (single or multiple) eigenvalue of the Laplace operator with the considered boundary conditions. It is then reasonable to use a rational approximant, in order to identify the singularities of the Helmholtz frequency response function. In particular, we introduce a reduced order model based

on the (single-point) Least Square (LS) Padé approximation technique, which gives a rational approximant from evaluations of the Helmholtz frequency response map and its derivatives only at one fixed center.

The single-point LS Padé technique is employed to approximate the frequency response map associated with various parametric time-harmonic acoustic wave problems (e.g., a transmission/reflection problem, a scattering problem and a problem in high-frequency regime). The Helmholtz equation with stochastic wavenumber is also considered.

2D numerical tests are performed, which confirm the effectiveness of the approximation method. Particular attention will be dedicated to a numerical example in high-frequency regime (where the singularities of the Helmholtz frequency response function are dense). In this case, the performance of the single-point LS Padé technique is unsatisfactory. A multi-point LS Padé approximant - based on the evaluations of the Helmholtz frequency response function and of its derivatives at multiple frequencies - is then considered.

S15.03 | Uncertainty quantification

Date: February 20, 2019

08:30-09:30

Room: HS 07

Sensitivity analysis for electrical detection of aortic dissection

Gian Marco Melito (*TU Graz, Austria*)

08:30

Vahid Badeli (*TU Graz, Austria*)

Alice Reinbacher-Köstinger (*TU Graz, Austria*)

Katrin Ellermann (*TU Graz, Austria*)

Numerical models often include a high degree of uncertainty. Uncertainty resides mainly in the input parameters of the model. This uncertainty results from errors in the measurement, in the lack of knowledge of the data, in assumptions made a priori on the model. In medical and patient-specific applications, uncertainty quantification and sensitivity analysis are indispensable in the process of diagnosis and decision-making.

We propose a method for the allocation of uncertainty in a model that simulates the measurement of the difference in electrical potential in the case of aortic dissection[1]. In particular, sensitivity analysis is divided into two steps.[2] The first step involves an initial screening using the Morris method, an OAT technical note. In the second step, we proceed with a global sensitivity analysis (GSA) of the model with a variance-based setting. From this setting, it is possible to develop a surrogate model of the Polynomial Chaos Expansion type. Subsequent post-processing on the coefficients of the PCE allows obtaining the Sobol Indices related to the GSA[3].

The numerical model initially includes a large number of input parameters grouped by data category: geometric properties, material properties. After the screening phase and having applied the prioritisation setting, we proceed with the analysis of the entire input space employing the polynomial expansion. This approach allows allocating more energy in the collection of sensitive data to the model and can significantly reduce the uncertainty of the output in question.

[1] Alimohammadi, M., Agu, O., Balabani, S., & Díaz-Zuccarini, V. (2014). Development of a patient-specific simulation tool to analyse aortic dissections: assessment of mixed patient-specific flow and pressure boundary conditions. *Medical engineering & physics*, 36(3), 275-284.

[2] Donders, W. P., Huberts, W., van de Vosse, F. N., & Delhaas, T. (2015). Personalization of models with many model parameters: an efficient sensitivity analysis approach. *International journal for numerical methods in biomedical engineering*, 31(10).

[3] Sudret, B. (2008). Global sensitivity analysis using polynomial chaos expansions. *Reliability Engineering & System Safety*, 93(7), 964-979.

On the calculation of a dry friction coefficient

Lukas Julian Oestringer (*Karlsruhe Institute of Technology, Germany*)

08:50

Carsten Proppe (*Karlsruhe Institute of Technology, Germany*)

Technical systems with friction are widespread in all kinds of applications. To simulate the frictional contact in these systems a large number of well studied static and dynamic friction laws is nowadays available. The models allow in general a good approximation of frictional phenomena, however, in most cases they lack completely of physical background. One possibility to get an insight into the actual contact situation is a simulation on the microscopic scale, which should be performed without simplifying the tangential contact by any kind of prescribed frictional law.

Therefore this contribution deals with the calculation of a physically motivated friction coefficient for the case of dry rough surfaces. Furthermore it investigates the influence of heat generation and velocity on the contact forces/area and as a result on the friction coefficient. A stochastic friction coefficient which only depends on physical properties is received. To this end the contact analysis is performed on a microscopic scale by using a half-space model. This includes the quasistatic solution of the thermo-elastic as well as the heat conduction equations and an elastic, perfectly plastic material law. The idea of “Bowden & Tabor” is picked up and leads finally to the physical friction coefficient.

Uncertainty quantification for optimal power flow problems

Tillmann Mühlpfordt (*Karlsruhe Institute of Technology, Germany*)

09:10

Veit Hagenmeyer (*Karlsruhe Institute of Technology, Germany*)

Timm Faulwasser (*Karlsruhe Institute of Technology, Germany*)

The need to de-carbonize the current energy infrastructure, and the increasing integration of renewables pose a number of difficult control problems. Among those, the optimal power flow (OPF) problem—i.e., the task to minimize power system operation costs while maintaining technical and network limitations—is key for operational planning of power systems. The influx of inherently volatile renewable energy sources calls for methods that allow to consider stochasticity directly in the OPF problem. Here, we present recent results on uncertainty quantification for OPF problems. Modeling uncertainties as second-order continuous random variables, we will show that the OPF problem subject to stochastic uncertainties can be posed as an infinite-dimensional L2-problem. A tractable and exact reformulation thereof can be obtained using polynomial chaos expansion (PCE), under mild assumptions. We will show advantageous features of PCE for OPF subject to stochastic uncertainties. For example, multivariate non-Gaussian uncertainties can be considered easily. We apply our findings to IEE test cases and demonstrate the efficacy of PCE applied to OPF subject to non-Gaussian stochastic uncertainties. Finally, we comment on recent progress on a Julia package for PCE.

S15.04 | Uncertainty quantification

Date: February 20, 2019

14:00-16:00

Room: HS 07

Scale switching computations for heterogeneous inelastic materials

Thilo Moshagen (*TU Braunschweig, Germany*)

14:00

Sadiq Sarfaraz (*TU Braunschweig, Germany*)

Bojana Rosic (*TU Braunschweig, Germany*)

Adnan Ibrahimbegovic (*University Technology Compiègne, France*)

Hermann G. Matthies (*TU Braunschweig, Germany*)

For computations involving heterogeneous inelastic materials it is often necessary to consider several scales, as it is not possible to compute the object of interest at the fine scale resolution required by the heterogeneity. For this purpose many proposals for multi-scale computations have been made. We will look at a two-scale transition in a general setting where both scales are also described probabilistically. By upscaling, using a fine-scale model the parameters for “homogenised” material models had been pre-identified.

We envision then two computational modes: one with such pre-identified homogenised material models, and the more expensive true two-scale computation used whenever the homogenised model is insufficient.

For this situation we examine thermodynamical quantities as computable criteria for locally estimating the modeling error in the homogenised material model. By providing a surrogate model for the criteria depending on load history, it is possible to adaptively decide - element by element - which computational path to use in that particular instance and location.

Performing Monte-Carlo-based Dynamic Event Trees (MCDET) for probabilistic analysis of complex dynamic systems

Nadine Berner (*Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Germany*)

14:20

Martina Kloos (*Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Germany*)

Josef Scheuer (*Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Germany*)

Jörg Peschke (*Gesellschaft für Anlagen- und Reaktorsicherheit (GRS) gGmbH, Germany*)

The analysis of complex dynamic systems in the presence of uncertainties influencing a system behavior, e.g. accident scenarios in nuclear power plants, is of fundamental interest for a safety assessment. The MCDET-analysis, as a combination of Monte Carlo (MC) simulation and the Dynamic Event Tree (DET) approach, enables to study the dynamic evolution of complex systems under the consideration of aleatory (stochastic) and epistemic (knowledge-based) uncertainties and to probabilistically assess the system behavior [1].

The MCDET-approach represents a probabilistic modeling concept by employing deterministic numerical simulation codes. The approach allows to cover a representative spectrum of event sequences resulting from the uncertain quantities taken into account and to provide an adequate probabilistic assessment of the consequences of critical event sequences. By starting a simulation sequence and initiating new simulation sequences as alternative system evolution paths due to random events, DET-structures of simulation paths are obtained. The DET-approach is generally

applied to uncertain quantities which are specified as discrete random variables (e.g. pump starts on demand yes/no). Uncertainties specified as continuous random variables (e.g. component failure time) are treated by MC-simulation. The advantages of the MCDET-approach over pure MC-simulation are its variance-reduction features in the probabilistic assessment and its significant reduction in computational time of the manifold simulation sequences. Even sequences with low occurrence probabilities are appropriately considered.

To efficiently perform the required multitude of simulation sequences, a scheduler approach has been developed that maps the DET-topology onto a hierarchical structure of simulation processes and stores the quantities of interest appropriately. The resulting hierarchical data base is used to investigate the spectrum of calculated simulation paths via statistical analysis methods to derive various probabilistic estimates, like means and conditional means, confidence intervals or conditional probability distributions of process quantities. Moreover, multivariate analysis approaches and basic machine learning concepts are applied to identify e.g. clusters of system states and sets of variables leading into critical system states.

The principles of the MCDET-approach in terms of probabilistic modeling, computational performance and statistical analysis are described using a simplified dynamic system of a hold-up tank. The analysis potential for the probabilistic evaluation of complex system behavior is discussed based on a fire event and on a station black-out accident in a nuclear power plant.

[1] M. Kloos, et al., MCDET: A Tool for Integrated Deterministic Probabilistic Safety Analyses, in *Modern Nuclear Energy Analysis Methods*, Vol. 1, ed. T. Aldemir, World Scientific Publishing (2018)

Optimal bounds for the probability of failure of sheet metal forming processes of DP steel

Niklas Miska (*Ruhr University Bochum, Germany*)

14:40

Daniel Balzani (*Ruhr University Bochum, Germany*)

Engineering designs and productions may be influenced by uncertainties for example due to natural variations, lack of knowledge, errors in measurements or any further reason. These uncertainties impede an efficient solution as large safety factors have to be applied. Therefore, a detailed analysis of the uncertainties is beneficial to reduce the arising costs while maintaining the level of safety. A suitable method is the Optimal Uncertainty Quantification framework [1], which allows the incorporation of uncertain parameters solely based on the available information. This allows for the calculation of the sharpest possible bounds on the probability of failure. As the framework is designed to treat each uncertain parameter as epistemic in the sense that full probability distributions are not known for the uncertain input parameters, we propose an extension to also incorporate aleatoric uncertainties. The capacity of this adapted framework is demonstrated for an example of a sheet metal forming process, which is subjected to aleatoric uncertainties describing the hardening behavior of the used steel [2], and epistemic uncertainties concerning e.g. structural parameters of the forming process, which may hardly be measurable. By comparing the resulting bounds for the probability of failure for different levels of knowledge of the epistemic parameters, the minimum required level of knowledge for meaningful bounds can be deduced.

[1] H. Owhadi, C. Scovel, T. Sullivan, M. McKerns, and M. Ortiz. Optimal uncertainty quantification. *SIAM Rev.*, 55:271-345, 2012.

[2] N. Miska and D. Balzani. A Method to Quantify Material Parameter Statistics Uncertainties Resulting from Microstructure Variation based on Artificial Microstructures. *Proceedings in Applied Mathematics and Mechanics*, 18, 2018 (accepted).

Numerical methods for density driven groundwater flow with uncertain data

Alexander Litvinenko (*King Abdullah University of Science and Technology, Saudi Arabia*) 15:00

Dmitry Logashenko (*King Abdullah University of Science and Technology, Saudi Arabia*)

Raul Tempone (*King Abdullah University of Science and Technology, Saudi Arabia*)

Gabriel Wittum (*King Abdullah University of Science and Technology, Saudi Arabia*)

David Keyes (*King Abdullah University of Science and Technology, Saudi Arabia*)

In many countries groundwater is the strategic reserve, which is used as a drinking water and as an irrigation resource. Therefore, accurate modeling of the pollution of the soil and groundwater is highly important. As a model we consider a density-driven groundwater flow problem with uncertain porosity and permeability. This problem may arise in geothermal reservoir simulation, natural saline-disposal basins, modeling of contaminant plumes and subsurface flow.

This strongly non-linear problem describes how salt or polluted water streams down building "fingers". The solving process requires a very fine unstructured mesh and, therefore, high computational resources. Therefore, we run the parallel multigrid solver UG4 (<https://github.com/UG4/ughub.wiki.git>) on Shaheen II supercomputer.

The parallelization is done in both - the physical space and in the stochastic space. The novelty of this work is the estimation of risks that the pollution will achieve a certain dangerous concentration at a given point. Additionally, we demonstrate how the multigrid UG4 solver can be run in a black-box fashion for testing different scenarios in density driven flow.

In the numerical section we solve Elder's problem in 2D and 3D domains, where unknown porosity and permeability are modeled by random fields. For approximations in the stochastic space we use the generalized polynomial chaos expansion. We compute different quantities of interest such as the mean, variance and exceedance probabilities. As a reference solution we use the solution, obtained by a quasi Monte Carlo method.

Literature

1. L. Giraldi, A. Litvinenko, D. Liu, H. G. Matthies, A. Nouy, To be or not to be intrusive? The solution of parametric and stochastic equations - the "plain vanilla" Galerkin case, *SIAM J. Sci. Comput.*, 36(6), A2720-A2744, 2014
2. W. Nowak, A. Litvinenko, Kriging accelerated by orders of magnitude: combining low-rank covariance approximations with FFT-techniques, *Mathematical Geosciences*, 2013, Vol. 45, Issue 4, pp 411-435
3. A. Litvinenko, HG Matthies, Sparse data representation of random fields, *PAMM: Proceedings in Applied Mathematics and Mechanics* 9 (1), 587-588, 2009
4. S. Reiter, A. Vogel, I. Heppner, M. Rupp, and G. Wittum, A massively parallel geometric multigrid solver on hierarchically distributed grids, *Computing and Visualization in Science*, 16(2013), pp. 151-164
5. A. Vogel, S. Reiter, M. Rupp, A. Nägel, and G. Wittum, UG 4: A novel flexible software system for simulating pde based models on high performance computers, *Computing and Visualization in Science*, 16 (2013), pp. 165-179.

Uncertainty propagation in a reinforced concrete model with localised failure

Simona Dobrilla (*TU Braunschweig, Germany, Université de Technologie de Compiègne, France*) 15:20

Noemi Friedman (*TU Braunschweig, Germany*)

Hermann G. Matthies (*TU Braunschweig, Germany*)

Adnan Ibrahimbegovic (*Université de Technologie de Compiègne, France*)

Addressing the structural durability challenges of concrete comes down to the problem of building models that can take into account complex mechanical phenomena, such as crack opening, bond-slip etc. Models capable of such representation are usually highly nonlinear and may be very sensitive to their material input parameters, which are often hard to estimate or they rely upon experiments. Therefore, they contain some inherent randomness which has to be incorporated from the beginning of the modelling process in order to identify how it propagates through the structural model response. In this work uncertainty propagation and bond-slip behaviour of a highly nonlinear model, which can take into account different failure mechanisms in reinforced concrete, are explored. Localised failure of concrete is modelled by a strong discontinuity approach and the material properties of bond-slip are considered as random fields. The aim is to quantify the uncertainty in the chosen nonlinear model in terms of providing a detailed description of localised failure of reinforced concrete pertaining to the crack spacing and opening.

Surrogate modelling for the global sensitivity analysis of problems with rapid local variations

Juan Manuel Lorenzi (*Technische Universität München, Germany*) 15:40

Sandra Döpking (*Freie Universität Berlin, Germany*)

Sebastian Matera (*Freie Universität Berlin, Germany*)

Surrogate modeling has become a popular tool in uncertainty quantification to lift the problem of repetitive, computationally expensive evaluations of a high fidelity model. Surrogate modeling becomes challenging when the underlying model shows locally rapid variations, e.g. if a materials model exhibits a phase transition within the parameter domain. We present a modification of the classical Shepard interpolation, which has been designed for such problems. In this approach, interpolation is achieved by blending local polynomial approximations based on the distances from the respective nodes. In order to exploit that, locally, rapid variations often appear in only a few directions, we replace the global distance metric by a local, node specific metric. We further introduce empirical local error estimates for each local polynomial and employ these to weight the different contributions at a query point. We demonstrate the approach on the global sensitivity analysis of a realistic stochastic model for CO oxidation, which has been parametrized using quantum-chemical methods. We find that we can obtain reasonably accurate estimates of the sensitivity indices already at a modest number of evaluations of the original high-fidelity model.

S15.05 | Uncertainty quantification

Date: February 20, 2019

16:30-18:30

Room: HS 07

Multifidelity reliability estimation

Carsten Proppe (*Karlsruhe Institute of Technology, Germany*)

16:30

Multi-fidelity estimation combines the output of simulation models of different approximation quality and from different sources in order to obtain efficient estimators for a quantity of interest. For Monte Carlo simulation, a multi-fidelity method based on control variates has been proposed in [1], where a model hierarchy is established based on the correlation of the low-fidelity models to a high-fidelity model. Moreover, an approach based on conditional probabilities for the quantity of interest between a high- and a low-fidelity model has been investigated in [2].

In this talk, a different approach for multi-fidelity reliability estimation will be presented, where the model hierarchy is based on f-divergences for the quantity of interest with respect to a high-fidelity model. To combine the results from the model hierarchy, fusion methods based on differences of the quantity of interest, on copula, and on conditional probabilities are compared. They are then combined with adaptive importance sampling and the moving particles method in order to yield efficient estimators for the probability of failure. The interaction between fusion and sampling will be especially highlighted.

Finally, the multi-fidelity reliability estimation methods are compared and critically assessed based on numerical experiments.

References:

- [1] B. Peherstorfer, K. Willcox, M. Gunzburger: Optimal Model Management for Multifidelity Monte Carlo Simulation. *SIAM Journal on Scientific Computing* 38(5), A3163-A3194, 2016
- [2] J. Biehler: Efficient Uncertainty Quantification for Large-Scale Biomechanical Models Using a Bayesian Multi-Fidelity Approach. Doctoral Thesis, TU Munich, Germany, 2016

Stochastic multi-level analysis of bone tissue

Sharana K. Shivanand (*TU Braunschweig, Germany*)

16:50

Bojana Rosic (*TU Braunschweig, Germany*)

Hermann G. Matthies (*TU Braunschweig, Germany*)

Human bone tissue is a typical example of material which exhibits randomness in the mechanical response due to an uncertain heterogeneous micro-structure. In order to develop an appropriate probabilistic macro-scale mathematical description, the essential step is to address the material as well as possible other sources of uncertainties (e.g. excitation's, change in geometry etc.) in the model. By extending already existing deterministic models derived from the Helmholtz free energy, the goal of this talk is to identify and quantify uncertainty in the system response. Due to essentially large number of parameters describing the material model, the process of obtaining the functional representation of the stochastic response is often proven to be computationally expensive. To relieve the computational demand, in this talk will be considered hybrid uncertainty quantification approaches that are based on the multi-element and multi-level approximations coming from the corresponding variational formulations.

Bayesian inversion for electrical impedance tomography

Michael Multerer (*Università della Svizzera Italiana, Switzerland*)

17:10

Robert Gantner (*Università della Svizzera Italiana, Switzerland*)

In this talk, we consider a Bayesian approach towards Electrical Impedance Tomography, where we are interested in computing moments, in particular the expectation, of the contour of an unknown inclusion, given noisy current measurements at the surface. By casting the forward problem into the framework of elliptic diffusion problems on random domains, we can solve it by means of the domain mapping method. This straightforwardly yields parametric regularity results for the system response, which we exploit to conduct a rigorous analysis of the posterior measure. The obtained results allow for the application of sophisticated quadrature methods for the approximation of quantities of interest. As an example of such a quadrature method, we consider an anisotropic sparse grid quadrature. Moreover, for the spatial discretization of the forward problem, we employ a fast boundary integral solver. Numerical examples are presented to illustrate the approach and validate the theoretical findings.

Bayesian analysis for Poisson-Boltzmann equation modeling electrical impedance tomography devices

Leila Taghizadeh (*TU Vienna, Austria*)

17:30

Clemens Heitzinger (*TU Vienna, Austria*)

Imaging the internal organs to diagnose diseases is one of the most important aspects of modern medicine. Tomography is one of the most important techniques in imaging, which could be used to monitor for internal bleeding, to screen for breast cancer, and to detect pulmonary emboli and blood clots in lungs. To this end, information about the distribution of electrical properties inside the body must be extracted by solving an ill-posed, nonlinear inverse problem. The corresponding tomography (forward) problem is called electrical impedance tomography (EIT) and it can be modeled by elliptic partial differential equations, namely the linear and nonlinear Poisson-Boltzmann equations, which are solved on a bounded and convex domain.

The domain of interest is a part of the body, which is equipped with electrodes attached to its surface. In an EIT sensor, small voltages are applied to the object of study through the electrodes and then the resulting current is measured on the boundaries. The goal of the EIT inverse problem is to extract the quantities of interest in the model, such as permittivities, charges, and sizes of inclusions or material layers in the main body. These parameters are of great importance in applications such as medicine to screen the interior body and to detect tumours or to determine body composition.

In this work, we estimate the mentioned geometrical and physical parameters as quantities of interest in the EIT inverse problem using Bayesian inversion methods. To this end, we use an adaptive Metropolis-Hastings (MH) algorithm. We present numerical results of the EIT forward and inverse problems considering eight contact electrodes attached to the surface of the body and operated in four different modes (voltage patterns or boundary conditions). The results for the inverse problem show good convergence of the Markov chains of the three parameters, and consequently accurate recovery of the parameters using Bayesian inversion based on the confidence intervals obtained for the parameters.

Furthermore, we prove well-definedness and well-posedness of the posterior measure for the Bayesian inversion for the EIT model by showing that the solution of the given model is bounded by a function of the parameters and that it is Lipschitz continuous with respect to the parameters.

Parameter estimation in a macroscopic production model based on a PDMP

Simone Göttlich (*University of Mannheim, Germany*)

17:50

Stephan Knapp (*University of Mannheim, Germany*)

Claudia Schillings (*University of Mannheim, Germany*)

We investigate parameter estimation in a production network model, which is based on a system of coupled ordinary and hyperbolic partial differential equations combined with time-dependent random capacity functions. The random capacity functions are piecewise constant in time and represent the capacity of a machine, reaching from zero, a machine failure, to maximal working capacity. A bidirectional relation between the production and the random capacity process characterizes the model. For this purpose, it is defined as a stochastic process and fits into the class of piecewise deterministic Markov processes (PDMPs).

The topology, production velocity and capacities are externally given and fixed parameters, whereas the dependence between machine failure probabilities and the production is incorporated as parameterized rate functions. These parameters are generally unknown and have to be estimated from time series of the production system. We present applicable methods to estimate these parameters and discuss numerical simulation results.

Bayesian inversion for nanoscale field-effect sensors using the stochastic drift-diffusion-Poisson-Boltzmann system

Amirreza Khodadadian (*Leibniz University of Hannover, Germany, Technical University of Vienna, Germany*)

18:10

Clemens Heitzinger (*Technical University of Vienna, Germany, Arizona State University, USA*)

Silicon nanowire sensors are highly miniaturized nanoscale devices used to detect the presence and concentration of various biological species such as cancer cells, DNA and miRNA molecules, and proteins. In these devices, the binding of target molecules to the receptors changes the charge concentration, which modulates the transducer. The drift-diffusion-Poisson-Boltzmann (DDPB) system is a comprehensive system of equations to model the electrical and electrochemical behavior of the devices.

Bayesian inversion serves to robustly estimate unknown model parameters such as diffusion coefficients and doping concentrations in order to obtain good agreement with experiments. Otherwise, these parameters cannot be measured directly or only with great experimental effort. More importantly, it also makes it possible to infer properties of the target molecules such as their charge and density.

In Metropolis-Hastings (MH) algorithms, the method proposal covariance must be manually tuned and has high autocorrelation. To overcome these deficiencies, we update the distribution according to the available samples (adaptive Metropolis) instead of using a fixed proposal distribution in each iteration. The adaptive method can be modified additionally by combining it with delayed rejection yielding the DRAM algorithm. In this algorithm, an alternative for the rejected candidate is proposed and the probability of this conditional acceptance is corrected.

In order to provide robust inverse modeling, we first validate the model (i.e., the DDPB system) and the simulations using experimental data. In order to study the effect of charged molecules on the nanowire, we estimated the molecule charge density. Then, we considered the effect of the doping concentration in a two-dimensional Bayesian inversion. Here, due to the well-localized probability density for each parameter, reliable information can be extracted. In addition to the mentioned physical parameters, we studied the effect of electron and hole mobilities in a four-dimensional Bayesian estimation. In the most complicated simulation, we have

estimated the probability density of the probe-target concentration. The results enable us to determine the device and molecule properties at the same time.

Finally, we have applied the parameters obtained by Bayesian inference to the DDPB system and again simulated the device current. The results show that the agreement with the experimental data has improved compared to the previous simulations, which indicates the effectiveness of the DRAM technique. In summary, this approach makes it possible to extract as much information as possible from nanoscale sensors in a rigorous manner.

S15.06 | Uncertainty quantification

Date: February 21, 2019

08:30-10:30

Room: HS 07

Multilevel and Multi-index Monte Carlo methods for the McKean-Vlasov equation

Raul Tempone (*KAUST, Saudi Arabia*)

08:30

In this talk, I will talk about our recent work where we address the approximation of functionals depending on a system of particles, described by stochastic differential equations (SDEs), in the mean-field limit when the number of particles is infinite. This problem is equivalent to estimating the weak solution of the limiting McKean-Vlasov SDE. To that end, our approach uses systems with finite numbers of particles and a time-stepping scheme. In this setting, there are two discretization parameters: the number of time steps and the number of particles. Based on these two parameters, we consider different variants of the Monte Carlo, Multilevel Monte Carlo (MLMC) and Multi-Index Monte Carlo methods and show that, based on some assumptions that are verified numerically, we are able to achieve a near-optimal work complexity in a typical setting.

Reference

"Multilevel and Multi-index Monte Carlo methods for the McKean-Vlasov equation", by Abdul-Lateef Haji-Ali, Raul Tempone, Preprint: arXiv:1610.09934, 2017. Published in Vol. 28, Issue 4, pp. 923-935. *Statistics and Computing*, 2018.

Higher-order methods for stochastic differential equations

Lisa Fischer (*Zuse Institute Berlin, Germany*)

09:10

Many biological processes such as gene expression are intrinsically stochastic in nature, and can be modelled by stochastic differential equations. Typically, model parameters like reaction propensities are unknown, and have to be estimated, e.g., using Bayesian inference. Also, often it is of interest to compute expectation values using (multilevel) Monte Carlo sampling, thus requiring the computation of many realizations by numerically approximating the involved SDEs. The discretization error of the numerical scheme induces bias in the computed Monte Carlo estimator. As the usually used numerical schemes, like Euler-Maruyama or Milstein, are low order, even reasonably coarse error bounds for the simulation are costly to achieve. In this talk we develop efficient higher order methods based on a Wong-Zakai approximation of Brownian motion combined with spectral deferred correction methods well known for the numerical solution of ordinary differential equations. We investigate the convergence order of the proposed method, and show numerical examples.

Joint work with Matthew R. Christian (UNC Chapel Hill), Sebastian Götschel (Zuse Institute Berlin) and Michael L. Minion (Lawrence Berkeley National Laboratory).

Well posedness and convergence analysis of the ensemble Kalman inversion

Dirk Blömker (*University of Augsburg, Germany*)

09:30

Claudia Schillings (*University of Mannheim, Germany*)

Philipp Wacker (*University of Erlangen, Germany*)

Simon Weissmann (*University of Mannheim, Germany*)

The ensemble Kalman filter (EnKF) is a widely used methodology for data assimilation problems and has been recently generalized to inverse problems as well. We present a complete analysis of the ensemble Kalman inversion with perturbed observations for fixed ensemble size when applied to linear inverse problems. The theoretical results are based on the analysis of the continuous time limit of the algorithm, i.e. a system of coupled stochastic differential equations. We show well-posedness of the scheme and present accuracy results of the EnKF estimate. We view the method as a derivative free optimization method for the least-squares misfit functional, which opens up the perspective to use the method in various areas of applications such as imaging, groundwater flow problems, biological problems as well as in the context of the training of neural networks.

Data assimilation using random set models: applications to dynamical system estimation

Truong-Vinh Hoang (*Technische Universität Braunschweig, Germany*)

09:50

Hermann G. Matthies (*Technische Universität Braunschweig, Germany*)

A random set is a generalization of a random variable, i.e. a set-valued random variable. The random set theory unifies other uncertainty descriptions such as the evidence theory, possibility theory and the set of probability distributions. It is hence a suitable framework to model the observation data that contains both noisy errors and coarsening effects, e.g. due to the accuracy of the measurement devices. The aim of this work is to develop a sequential data assimilation method that can account for coarsening and noisy measurements. To fuse prior and data induced random sets we use the Dempster's rule of combination developed in the evidence theory as an inference rule. A direct evaluation of the posterior random set might be unpractical. We approximate the posterior random set by a random finite set whose domain is the set of samples generated using a proposed probability distribution. We use the capacity transform density function of the posterior random set for this proposed distribution. This function has a special property: it is the posterior density function yielded by Bayesian inference of the capacity transform density function of the prior random set. Thanks to that property, the Markov Chain Monte-Carlo algorithms can be applied. The developed method is then applied to a dynamical problem. We show that when the data are sufficiently large, the posterior random set becomes a random variable.

Probabilistic numerics and randomised Bayesian inverse problems

Jon Cockayne (*University of Warwick, UK*)

10:10

Mark Girolami (*Imperial College London, UK, Alan Turing Institute, UK*)

Han Cheng Lie (*Freie Universität Berlin, Germany, Zuse Institute Berlin, Germany*)

Chris Oates (*Alan Turing Institute, UK, Newcastle University, UK*)

T. J. Sullivan (*Freie Universität Berlin, Germany, Zuse Institute Berlin, Germany*)

Aretha Teckentrup (*University of Edinburgh, UK*)

Probabilistic inference perspectives on numerical tasks such as quadrature and the solution of differential equations have received renewed attention in recent years. Such methods offer a statistical characterisation of discretisation uncertainty suitable for incorporation in larger inferential pipelines. We will review some recent contributions in this area, in particular what it means for a numerical method to be probabilistic and to be Bayesian; how such Bayesian numerical methods can be aggregated into complex pipelines; and how the use of such random forward models affects the accuracy of the computed posterior.

S15.07 | Uncertainty quantification

Date: February 21, 2019

14:00-16:00

Room: HS 07

Stochastic approximation for PDE constrained optimization under uncertainty

Caroline Geiersbach (*University of Vienna, Austria*)

14:00

Georg Pflug (*University of Vienna, Austria*)

Models incorporating uncertain inputs, such as random forces or material properties, have been of increasing interest in PDE constrained optimization. Even though stochastic approximation has a rich history, dating back to a groundbreaking paper by Robbins and Monro in 1951, it has been unexploited in this field. In this talk, we present an efficient iterative method for solving problems with uncertainty in the PDE constraint. Iterations make use of a stochastic gradient, or a function approximating the gradient of the objective functional. We will demonstrate convergence for problems in Hilbert spaces and discuss aspects of efficiency and complexity. The approach will be demonstrated on a model problem with random elliptic PDE constraints.

Variational Monte Carlo - bridging concepts of machine learning and high dimensional partial differential equations

Martin Eigel (*Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany*)

14:20

Reinhold Schneider (*Technische Universität Berlin, Germany*)

Philipp Trunschke (*Technische Universität Berlin, Germany*)

Sebastian Wolf (*Technische Universität Berlin, Germany*)

A statistical learning approach for parametric PDEs related to Uncertainty Quantification is derived. The method is based on the minimization of an empirical risk on a selected model class and it is shown to be applicable to a broad range of problems. A general unified convergence analysis is derived, which takes into account the approximation and the statistical errors. By this, a combination of theoretical results from numerical analysis and statistics is obtained. Numerical experiments illustrate the performance of the method with the model class of hierarchical tensors.

Uncertainty quantification for the inflow control in hyperbolic supply systems with uncertain demand

Simone Göttlich (*University of Mannheim, Germany*)

14:40

Oliver Kolb (*University of Mannheim, Germany*)

Kerstin Lux (*University of Mannheim, Germany*)

In this talk, we address the challenging task of setting up an optimal production plan taking into account uncertain demand. We use uncertainty quantification for an adaptation to different levels of risk aversion.

The supply system is represented by a hyperbolic conservation law and the uncertain demand stream is captured by an Ornstein-Uhlenbeck process. With a model predictive control approach, we determine the optimal inflow depending on the producer's risk preferences. The resulting output is intended to optimally match the stochastic demand for the given risk criteria. In a numerical simulation study, we analyze the effect of different risk levels on the optimal output.

Efficient yield optimization of electromagnetic devices

Mona Fuhrländer (*TU Darmstadt, Germany*)

15:00

Sebastian Schöps (*TU Darmstadt, Germany*)

Uncertainty quantification and optimization under uncertainty become increasingly important in the context of electromagnetic field simulation since devices are developed closer to their physical limits. Deviations in the manufacturing process of electronic components may lead to rejections due to malfunctioning. The probability that a product fulfills its performance specifications is called the yield. We aim to maximize the yield, which corresponds to minimizing the failure probability. Thereby the quality of the electrical device is improved and time and resources can be saved.

The uncertain design variables are modeled as random variables with a known probability density function. The performance specifications involve the partial differential equations describing the electromagnetic field, i.e., Maxwell's equations in time or frequency domain.

In the case of realistic problems, the yield can not be calculated analytically and discretization methods are employed, e.g. the finite element method for space discretization. Every function evaluation in the optimization involves hundreds of calls of the finite element solver, which is very time consuming. Thus, an efficient approximation is required to estimate the yield. In this work we present an approach, combining Monte Carlo and Stochastic Collocation. In order to optimize the yield we investigated different gradient based optimization approaches.

Acknowledgements: This work is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

Kriging assisted Particle Swarm Optimization for efficient non-intrusive interval analysis

Noemie Le Carrer (*University of Liverpool, United Kingdom*)

15:20

David Moens (*KU Leuven, Belgium*)

Matthias Faes (*KU Leuven, Belgium*)

Recent developments in interval analysis introduced highly efficient procedures for the propagation of interval uncertainty in numerical models [1, 2]. However very powerful, these methods require a modification of the underlying numerical code, which is in an industrial context not always feasible or desirable. Therefore, often global optimization algorithms are used to actively search the hyper-rectangular space bounded by the parameter intervals for those realizations that yield extreme model responses. While being very accurate, such an approach typically requires a large number of full model evaluations, resulting in a high computational cost, especially for strong non-linear numerical models. This paper presents an efficient procedure for the propagation of intervals through such strong non-linear numerical models in a non-intrusive setting using a combination of adaptive Kriging refinement and Particle Swarm Optimization (PSO). Based on an initial sparse large space filling design, a Kriging model is trained to represent the full numerical model approximately. The Kriging estimator is then optimized towards the global extrema of the model by iteratively enriching the design based on PSO estimations of the

global extrema, taking the variance of the estimator into account (as e.g., shown in [3]). The method is illustrated on well-known benchmark test functions, and it is shown that by combining Kriging with PSO, the total number of full model evaluations is reduced drastically as compared to performing global optimization directly on the numerical model, while maintaining accurate results.

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Robust aerodynamic design optimization via primal-dual aggregation method

Emre Özkaya (*TU Kaiserslautern, Germany*)

15:40

Nicolas R. Gauger (*TU Kaiserslautern, Germany*)

Robust aerodynamic design optimization using Euler or Navier-Stokes equations can be computationally very challenging since the computational effort for the underlying flow simulations is usually very high. For these problems, especially with the increasing number of design parameters, evaluating statistical quantities such as variation or mean in a Monte-Carlo or quasi Monte-Carlo framework is impractical. One way of overcoming this problem is by constructing approximation models, known as surrogate models that mimic the behavior of the underlying simulation as closely as possible while being computationally cheap. In this way, evaluation of statistical quantities or even worst case scenarios becomes feasible in robust optimization.

Since surrogate models are constructed using a data-driven approach, a training data set is necessary to adjust the model parameters. The training data set should be ideally large to avoid high generalization errors. In an aerodynamic design optimization framework, however, the number of samples that can be generated to train the surrogate model is very limited due to restricted computational resources. On the other hand, recent achievements in adjoint methods has made the evaluation of gradient information possible for a wide variety of aerodynamic simulations and at a reasonable computational cost. Therefore, using an adjoint solver, the amount of data that is collected in the Design of Experiment (DoE) stage can be significantly increased. The key idea is then to use these richer data sets while training a surrogate model, which achieves a higher model accuracy and a lower generalization error using the same number of training samples.

In the present talk, we present a novel aggregation method, which is in essence a boosting method combining two different surrogate models with a spatially varying weight function. The main advantage of the aggregation method is that it enables the state of the art surrogate models to incorporate extra gradient information without causing overfitting problems. Therefore, accurate surrogate models with relatively large number of design parameters can be constructed using small data sets. Furthermore, the computational effort required to train the model is significantly lower than the standard models using gradient information such as the Gradient Enhanced Kriging method. We also present results from several benchmark aerodynamic design optimization problems showing the efficiency and the robustness of the new method.

S15.08 | Uncertainty quantification

Date: February 21, 2019

17:40-18:40

Room: HS 07

Uncertainty quantification and prediction error meta classification in semantic segmentation with deep neural networks

Matthias Rottmann (*University of Wuppertal, Germany*)

17:40

Pascal Colling (*University of Wuppertal, Germany*)

Thomas-Paul Hack (*Leipzig University, Germany*)

Fabian Hüger (*Volkswagen Group Research, Germany*)

Peter Schlicht (*Volkswagen Group Research, Germany*)

Hanno Gottschalk (*University of Wuppertal, Germany*)

We present a method that "meta" classifies whether segments predicted by a semantic segmentation neural network intersect with the ground truth. To this end, we employ measures of dispersion for predicted pixel-wise class probability distributions, like classification entropy, that yield heat maps of the input scene's size. We aggregate these dispersion measures segment-wise and derive metrics that are well-correlated with the segment-wise intersection over union (IoU, also known as Jaccard Index) of prediction and ground truth. In our tests, we use two publicly available DeepLabv3+ networks (pre-trained on the Cityscapes data set) and analyze the predictive power of different metrics and different sets of metrics. To this avail, we compute logistic LASSO regression fits for the task of classifying $\text{IoU}=0$ vs. $\text{IoU}>0$ per segment and obtain classification rates of up to 81.91% and AUROC values of up to 87.71% without the incorporation of advanced techniques like Monte-Carlo dropout. We complement these tests with linear regression fits to predict the segment-wise IoU for modelling uncertainty on segment level and obtain prediction standard deviations of down to 0.130 as well as R^2 values of up to 81.48%. We show that these results clearly outperform single-metric baseline approaches.

Bayesian multi-scale analysis of mechanical structures

Bojana Rosic (*TU Braunschweig, Germany*)

18:00

Muhammad Sarfaraz (*TU Braunschweig, Germany*)

Sharana K. Shivanand (*TU Braunschweig, Germany*)

Ameya Reege (*RWTH Aachen University, Germany*)

Hermann G. Matthies (*TU Braunschweig, Germany*)

Human bone tissue, aero-gels and concrete are typical examples of material which exhibits randomness in the mechanical response due to an uncertain heterogeneous micro-structure. In order to develop an appropriate probabilistic macro-scale mathematical description, the essential step is to address the material as well as possible other sources of uncertainties in the model. By extending already existing deterministic generalised continuum models derived from Helmholtz free energy and the dissipation functions characterising ductile or quasi-brittle behaviour, the goal of this talk is to identify and quantify uncertainty in the macro-scale response from a Bayesian probabilistic point of view. This requires an efficient algorithm for solving possibly high dimensional probabilistic forward problems on a micro-scale level. An emergent idea is to propagate parametric uncertainties through the model in a hierarchical manner in which the solution of the corresponding differential equations is represented by a set of stochastic basis polynomials in a low-rank format. Here will be discussed some of novel approaches to achieve this goal.

Causality and Bayesian network PDEs for multiscale representations of porous media

Eric Joseph Hall (*RWTH Aachen University, Germany*)

18:20

Kimoon Um (*Stanford University, USA*)

Markos Katsoulakis (*University of Massachusetts Amherst, USA*)

Daniel Tartakovsky (*Stanford University, USA*)

Hierarchical porous media that feature properties and processes at multiple scales arise in many engineering applications including the design of novel materials for energy storage devices. Microscopic (pore-scale) properties of the media impact their macroscopic (continuum- or Darcy-scale) counterparts and understanding the relationships between processes on these two scales is essential for informing engineering decision tasks. However, microscopic properties typically exhibit complex statistical correlations that present challenges for the estimation of macroscopic quantities of interest (QoIs), e.g., global sensitivity analysis (GSA) of macroscopic QoIs with respect to microscopic material properties that respect structural constraints. We present a systematic framework for building correlations into stochastic multiscale models through Bayesian networks. This allows us to construct the joint probability density function (PDF) of model parameters through causal relationships that emulate engineering processes related to the design of hierarchical nanoporous materials. Such PDFs also serve as input for the forward propagation of parametric uncertainty; our findings indicate that the inclusion of causal relationships impacts predictions of macroscopic QoIs. To assess the impact of correlations and causal relationships between microscopic parameters on macroscopic material properties, we use a moment-independent GSA based on the differential mutual information. Our GSA accounts for the correlated inputs and complex non-Gaussian QoIs. The global sensitivity indices are used to rank the effect of uncertainty in microscopic parameters on macroscopic QoIs, to quantify the impact of causality on the multiscale model's predictions, and to provide physical interpretations of these results for hierarchical nanoporous materials.

S15.09 | Uncertainty quantification

Date: February 22, 2019

08:30-10:30

Room: HS 07

Low-rank approximations for fuzzy-stochastic models

Dieter Moser (*RWTH Aachen University, Germany*)

08:30

Lars Grasedyck (*RWTH Aachen University, Germany*)

Robert Gruhlke (*WIAS, Germany*)

Martin Eigel (*WIAS, Germany*)

In the case where sufficient knowledge is missing to model a problem by means of stochastic distribution functions, two ways of argumentation open up. The first way is to argue that physical systems tend to maximize the entropy and, therefore, it is sensible to choose e.g. a uniform distribution, when only the possible range of the variable is given. As this argument is valid for many situations, it is also questionable for situations where for instance the parameter is known to take one of two possible values with unknown probability. Arguably, in these cases a non-stochastic model or a combination of a stochastic and a non-stochastic model may be more suited. One non-stochastic way to model the problem is to employ the fuzzy framework. In this talk we briefly introduce the fuzzy framework. Then, based on an example we compare the fuzzy-stochastic approach to a purely stochastic approach. In both cases it is helpful and

often necessary to have a surrogate model to cope with the arising computational effort. Thus, the application of a low-rank approximation, namely the hierarchical Tucker format, for both approaches will be addressed.

Reliability analysis for a polymorphic uncertainty model of heterogeneous materials using a domain decomposition approach

Tom Lahmer (*Bauhaus Universität Weimar, Germany*)

08:50

Albrecht Schmidt (*Bauhaus Universität Weimar, Germany*)

Carsten Könke (*Bauhaus Universität Weimar, Germany*)

Realistic analyses require appropriate models of uncertain input data. Polymorphic uncertainty approaches combine basic uncertainty models into one parameter, like a fuzzy random variable describing a material parameter [1]. Heterogeneous materials in geotechnical applications show spatial variation which are usually described by random fields (RF). RFs are characterized by an auto-correlation structure, whereas material interdependencies can be taken into account using cross-correlated RFs [2]. Usually, these RF parameters associated with auto- and cross-correlations are only vaguely known. Therefore, in the presented paper, they are described by convex fuzzy sets. The utilization of this polymorphic uncertainty model on large 3D finite element models leads to computational demanding computations. This issue can be tackled using a domain decomposition (DD) approach reducing the stochastic dimensionality by a parallelized execution off subdomain problems. The DD approach reported in [4, 5], utilizing a subdomain based stochastic surrogate model, is enhanced for a reliability analysis estimating failure probabilities. The suggested polymorphic material description using the RF parameter fuzzy sets as an input yields failure probability fuzzy sets as the results. A hydro-mechanical coupled system of a masonry gravity dam, implemented as finite element model, serves as an application example [3]. Results are shown for a traditional non-DD and the proposed DD approach comparing both the accuracy of estimated failure probabilities and the computational efficiency.

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A fuzzy uncertainty model for analytical and numerical homogenization of transversely fiber reinforced plastics

Ismail Caylak (*Paderborn University, Germany*)

09:10

Eduard Penner (*Paderborn University, Germany*)

Alexander Henkes (*Paderborn University, Germany*)

Rolf Mahnken (*Paderborn University, Germany*)

Lightweight structures, such as fiber reinforced plastics (FRP), become increasingly important due to their excellent mechanical and lightweight properties. The manufacturing process results

in uncertain material properties of FRP. In addition, there are measurement errors and missing or incomplete information on material properties. In scientific works, a distinction is often made between aleatoric and epistemic uncertainty. Aleatoric uncertainty is presumed to be the intrinsic randomness of a phenomenon. On the other hand, epistemic uncertainty is the vagueness in a system definition due to subjectivity, simplification and incomplete knowledge that can be modeled with fuzzy methods based on the fuzzy set theory.

It is well known that composites' microstructures are heterogeneous with at least two constituents of different material properties on the micro-scale. Instead of developing a macroscopic phenomenological constitutive law, it is more accurate to develop a two-scale microscopic model based on analytical and numerical homogenization methods to predict their effective properties. Analytical mean-field methods, such as Mori-Tanaka, self-consistent and interaction direct derivative, are based on the Eshelby solution to an ellipsoidal inclusion embedded in an infinite matrix. In numerical homogenization methods, such as FE², a representative volume element (RVE) of the microstructure at each point of the macrostructure is attached.

This contribution presents a framework of a fuzzy uncertainty model for analytical and numerical homogenizations of transversely FRP. Epistemic material parameters are defined as design variables and are modeled as fuzzy sets. An underlying optimization problem for the fuzzy analysis is approximated by alpha-level discretization techniques, resulting into a separation of minimum and maximum problems. Finally, results for analytical and numerical homogenizations are compared.

S16 | Nonsmooth optimization II

Organiser: Christian Kirches (*Technische Universität Braunschweig, Germany*)
Christian Clason (*University of Duisburg-Essen, Germany*)

S16.01 | Experiment design

Date: February 20, 2019
Room: HS 06

08:30-09:30

First-order methods for regularized optimal experimental design problems

Roland Herzog (*TU Chemnitz, Germany*)
Eric Legler (*TU Chemnitz, Germany*)

08:30

The task of parameter identification of a certain model by carrying out experiments is closely connected to the question of finding the most informative experimental conditions. The computation of these conditions leads to so-called Optimal Experimental Design problems.

These can be cast in the form $\min F(\Lambda(w)) + G(w)$, where $w \in C^*(X)$ is a measure, F and G are convex functionals and Λ is a linear operator. Specifically, G is the indicator function of the convex set of feasible weights and F corresponds to a design criterion which is assumed to be differentiable.

In our approach, we add a Tikhonov term and obtain a problem with a density w in the Hilbert space $L^2(X)$ instead. We will consider problems where the set of feasible weights does or does not contain pointwise upper bounds. After discretization we compare various first-order methods of proximal gradient type by applying them to the problem at hand.

Sensitivity analysis of elastoplastic structures and application to optimal specimen design

Jan Liedmann (*TU Dortmund University, Germany*)

08:50

Franz-Joseph Barthold (*TU Dortmund University, Germany*)

The aim of this paper is to improve the shape of specimens for biaxial experiments w.r.t. optimal stress states, characterized by the stress triaxiality. Gradient based optimisation strategies are used to achieve this goal. Thus, it is crucial to know how the stress state changes if the geometric shape of the specimen is varied.

Design sensitivity analysis (DSA) of the stress triaxiality gives an adequate answer to this question. The variational approach, proposed in [1], based on an enhanced kinematic concept that offers a rigorous separation of structural and physical quantities, provides exact gradient information efficiently with moderate effort. Additionally, it allows simultaneous computation of stress states and sensitivities within a finite element framework, c.f. [2]. Considering elastoplastic material behaviour the deformation history as well as its sensitivity has to be taken into account, c.f. e.g. [3].

In order to apply the method mentioned above to real world materials, in a first step a parameter identification (PI) has been performed to fit the material parameters to the chosen numerical model. For this purpose, sensitivity information w.r.t. material properties have been computed using the variational approach mentioned above.

Improved specimen for biaxial experiments have been developed in [4] and are taken as basis in this work. The optimisation problem to be solved is to maximise the stress triaxiality by changing the geometry of the specimen.

Numerical and algorithmic implementation is presented and results are shown for chosen specimens.

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Oblique projections and optimal actuator placement

Kevin Sturm (*TU Wien, Austria*)

09:10

Sergio S. Rodrigues (*TU Wien, Austria*)

In this talk we discuss an optimal actuator placement problem in 1D arising from the maximisation of the operator norm of oblique projections (nonorthogonal projections) in Hilbert spaces. These particular oblique projections play a crucial role in recently proposed stabilisation techniques for parabolic equations. The optimisation problem is nonsmooth and nonconvex and depends on the chosen boundary condition. We prove that for the Neumann and Dirichlet Laplacian symmetric actuator positions are always stationary points.

In case of two actuators we give a complete characterisation of the optimal actuator location problem and provide explicit formulas. We show that in case of Dirichlet boundary conditions there exists a unique global solution which is symmetric. In contrast, for Neumann boundary conditions we show that we have infinitely many globally optimal actuator positions and each of them is symmetric.

In the final part of the paper we provide numerical results supporting our theoretical findings.

S16.02 | Shape & material optimization I

Date: February 20, 2019

14:00-16:00

Room: HS 06

Free material optimization of multilayer composite materials

Simon Loske (*TU Dortmund, Germany*)

14:00

Franz-Joseph Barthold (*TU Dortmund, Germany*)

The use of composite materials in various types of devices has increased steadily in the past decades. Hence it is worth investigating into the structural behaviour of these materials. The optimization of stacking sequences in multilayer composite materials opens a large field of improvements in industrial applications of composite materials. The center of investigation is set on fiber reinforced laminate plies, which are examined in the case of linear anisotropic theory of elasticity. The natural way of modelling typical domains of application is the deployment of geometrical non-linear shell elements.

One very auspicious way for optimization of these laminates is the implementation of Free Material Optimization [1].

In these optimization procedures arbitrary values of parameters of the elasticity matrix are obtained under constraints which only claim the elasticity matrix to be symmetric and positive

semi definite. Also the trace of the elasticity matrix is restricted to avoid the total stiffness of the material to get unnaturally large. The sensitivity information are received by the variational approach for sensitivity analysis [2] which represents the most efficient known way of computing sensitivity information.

The Free Material Optimization for multilayer materials yields an optimal distribution of material parameters in each single layer of the stacked ply that can be taken into account for further optimization procedures to choose the best fitting material for plies of the considered stack.

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Automatic shape optimization of a 180-degree elbow for pressure loss minimization

Eman Bagheri (*FAU Erlangen, Germany*)

14:20

Alexander Lodermeier (*FAU Erlangen, Germany*)

Andreas Logdesser (*FAU Erlangen, Germany*)

Stefan Becker (*FAU Erlangen, Germany*)

The application of the adjoint-based shape optimization in fluid mechanics has increasingly received more attention in the past few years. However, the validity of the optimization results is in question due to uncertainties of the underlying turbulence models and further simplifications made in the adjoint equations.

In this work, we present the results of the discrete adjoint shape optimization of a 180-degree elbow for the purpose of pressure loss minimization. Additionally, a test-rig was designed to validate the outcome of the simulation. For this purpose, the RANS equations with the $k-\omega$ -SST model are solved to obtain the mean flow fields. The objective function to be minimized is defined as the field integral of the entropy generation due to viscous dissipations. The gradient of the objective function is obtained using the discrete adjoint solver in the open source software SU². The algorithmic differentiation incorporated in SU² provides an accurate and robust procedure to compute the gradient of the discrete objective function without having to make any simplifications such as frozen turbulence assumption. In each optimization cycle, the calculated gradient is fed to the conjugate gradient optimizer and the grid is deformed according to the current design until the optimization process terminates. The surface of the enhanced geometry is then derived from the computational grid and the optimal design is fabricated using the 3D printing technology.

The optimal geometry is verified against the baseline design and the resulting experimental data confirms the reliability of the numerical simulations. The optimization procedure successfully decreases the radial pressure gradient inside the elbow thereby minimizing the energy of the dean vortices and removing the recirculation bubble downstream of the bend. As a result, the experimental study of the optimal design shows a significant pressure loss improvement over a wide range of Reynolds numbers. The result of this optimization problem paves the way for designing highly-efficient heat exchangers. Moreover, this study highlights the feasibility of the discrete adjoint shape optimization for a broader variety of problems in industrial applications. Consequently, the overall efficiency of a complicated system can be improved drastically only by making minor geometric modifications to its critical components. Although we have performed an unconstrained optimization for this test case, appropriate geometric constraints may be needed in practical applications in order to obtain less complex geometries suitable for conventional manufacturing methods.

Controlling physical properties on interfaces using parametrised level set methods and extended finite element method

Felix Wohlgemuth (*TU Dortmund, Germany*)

14:40

Franz-Joseph Barthold (*TU Dortmund, Germany*)

The stress field information states a main point of interest, when regarding structural optimisation of bimaterial structures. The introduction of stress criteria along the volume is crucial in the development of new designs. In the case of bimaterials the stress field along the interface deserves additional attention e.g. to prevent delamination. Tracing the interface through shape optimisation in CAD-based methods is rather expensive due to the high cost in remeshing techniques. Therefore level set methods with fixed background meshes are used as in [1].

In this work an approach for controlling strains and stresses on the interface in a framework of shape optimisation is introduced. The geometry description is managed by parametrised level set functions and a sub-meshing technique is coupled with the extended finite element method. The parametrisation with superellipses allows to reduce the number of design variables to a minimum of six variables per introduced ellipse while holding up a sufficient precision in the geometry description (see [2]). Moreover, it simplifies the shape derivatives as it provides an implicit description for the moving interfaces. The sub-meshing technique makes it possible to keep existing strategies from homogeneous structures and to transform them on a discontinuous material using enriched shape functions provided by the standard extended finite element method (see [3]). Shape sensitivities are evaluated on the sub-elements and extrapolated to the interface introducing pseudo nodes. The sensitivity information of the stress field among these pseudo nodes can be used in the framework of stress minimisation as well as for a side condition in a volume minimisation setup. Results are discussed regarding algorithmic difficulties and inaccuracies in the sensitivity analysis due to ill-conditioning and insufficient mapping assumptions.

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Calibration of model coefficients of an extended eddy viscosity turbulence model for vortical flows

Noemi Friedman (*TU Braunschweig, Germany*)

15:00

Elmar Zander (*TU Braunschweig, Germany*)

Gokul Subbian (*TU Braunschweig, Germany*)

In this contribution the two-equation Menter-Shear Stress Transport turbulence model is considered. While the model is relatively robust and requires much less computational resources than more sophisticated approaches as Reynolds Stress Models, unfortunately it can purely model complex flow phenomenon such as vortical flows. Here a combination of different correction models are investigated and calibrated to overcome this drawback of the model using experimental data of different benchmark problems. The calibration is carried out by trying to fit the model responses — such as velocity field, Reynold stresses, lift and pressure coefficients

to these experimental data. The inverse problem is carried out by first finding an optimal surrogate model replacing the flow simulations. Conventional optimization techniques and Bayesian update was used for elaborating an optimal correction model suitable for modeling complex flow phenomenon.

Comprehensive optimization of frame structures

Alexander Keller (*Karlsruhe Institute of Technology, Germany*)

15:20

Ingo Muench (*Karlsruhe Institute of Technology, Germany*)

Werner Wagner (*Karlsruhe Institute of Technology, Germany*)

Structural design optimization problems are typically characterized by their large numbers of design variables and constraints, high degree of non-linearity and multitude of local minima. Additionally, there are often contradictory optimization objectives, e.g., minimizing mass and maximize stiffness of a structure. Thus, an engineer has to face are great demands on the algorithms used.

For the comprehensive optimization of frame structures in civil engineering, we present a software tool at a high level of automatization. It decomposes the optimization task into two stages: the topology optimization and the shape optimization including sizing. The use of different optimization algorithms adjusted to the requirements of each stage is expedient. First, a phase field model is used to evolve a topology as basic design. It starts with a uniformly filled region of substance bounded by the maximum dimensions. It has the objective to find a load bearing topology with a homogeneous stress field. It determines the relevant characteristics of a structure such as the number of beams and the approximate position of nodes.

Next, an interface picks up this design to set up a simplified beam model. The model reduction is performed automatically based on image processing algorithms without the intervention of an engineer.

The subsequent shape optimization with an Evolutionary Algorithm considers the normative constraints with cross section of members, exact position of nodes and the connection type of members as simultaneous optimization variables. The latter determines the arrangement of rigid and pinned connections within the frame structure. Especially deformation restricted optimization problems have advantages by activating the bending load capacity of members. However, in some cases, it results in increased stresses and thus larger profiles. If the joints are optimally arranged in the structure, smaller deformations are achieved with less total weight. We present examples to explain the proposed double-stage optimization yielding globally optimized frame structures.

Load optimisation for air bending in the context of damage reduction

Fabian Guhr (*Technische Universität Dortmund, Germany*)

15:40

Franz-Joseph Barthold (*Technische Universität Dortmund, Germany*)

Rickmer Meya (*Technische Universität Dortmund, Germany*)

A. Erman Tekkaya (*Technische Universität Dortmund, Germany*)

Forming in the industrial setting requires precise knowledge of the underlying mechanical effects to generate specific components with their requested characteristics. In order to further expand the possibilities of given forming processes, the material properties have to be utilised to their full potential. A critical property that leads to macroscopic cracks and fractures, which are to be avoided, is the accumulation of damage during the forming process. As such, the growth of damage has to be reduced in order to create more durable parts or allow larger deformations. Research for air bending has shown that the superposition of additional pressure forces in the critical region of the forming process, by means of an elastomer cushion (elastomer bending), yields less microscopic defects and a reduced damage state in the final component, see e.g. [1].

By replacing the elastomer cushion with nodal pressure forces, these applied forces can be used as the design for mathematical optimisation and allow for the necessary load optimisation. Since the final shape of the load optimised component shall remain close to the original profile, for sake of comparison, the objective function is chosen to be a least square problem type between the original displacement field and the displacement field for the current design. Incorporating the triaxiality, a measure of stress-state to identify critical damage areas, allows the generation of optimal loads to reduce damage growth in the critical domains of the bending simulation. Furthermore, this optimisation concept allows the enhancement of the elastomer bending by generating optimal loads to induce homogenised triaxiality values in the bending area, such that critical loads are distributed over larger regions which circumvent critical stress spikes to focus in a small domain and furthermore generate identical component behaviour at the forming area. The concept of load optimisation has been shown in e.g. [2] with a variational aspect in mind. This work however is done purely numerical, where Abaqus is used as a solver with the data being parsed via Python to Matlab for the mathematical optimisation.

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S16.03 | Shape & material optimization II

Date: February 20, 2019

16:30-18:30

Room: HS 06

Metamodel assisted optimization of glued laminated timber beams by using metaheuristic algorithms

Sebastian Pech (*TU Wien - Vienna University of Technology, Austria*)

16:30

Georg Kandler (*TU Wien - Vienna University of Technology, Austria*)

Markus Lukacevic (*TU Wien - Vienna University of Technology, Austria*)

Josef Füssl (*TU Wien - Vienna University of Technology, Austria*)

An efficient use of the raw material in glued laminated timber (GLT) beams is commonly achieved by inserting lamellas of lower quality in less stressed areas, usually in the middle of a beam. But, this rather simple method leaves room for improvement. In particular, the morphology of a board and its location in the beam setup is significant, since only this information and the actual loading situation allows a proper evaluation of weaknesses. Therefore, a new optimization method was developed, able to take mechanical property distributions as well as the occurring stress states within each wooden board into account.

Subsequent to an automatic knot reconstruction and determination of effective local stiffness distributions of all boards, the beams are analyzed using a finite element (FE) model. This information is further exploited to find optimal beam setups out of a sample of boards. However, as the complexity of this optimization task quickly increases with the number of boards, metaheuristic optimization algorithms were developed. Additionally, the evaluation of the computationally expensive FE model is bypassed by a metamodel, capable of approximating the desired performance parameter of any beam. Comparing the various optimization approaches to common GLT beam production methods, maximum deflection can be reduced by 15-20%.

Shape optimization of bridge decks considering the Vortex-induced vibration phenomena

Zouhour Jaouadi (*Bauhaus Universität Weimar, Germany*)

16:50

Tajammal Abbas (*Bauhaus Universität Weimar, Germany*)

Guido Morgenthal (*Bauhaus Universität Weimar, Germany*)

Tom Lahmer (*Bauhaus Universität Weimar, Germany*)

Due to the effect of the wind that can be harmful and causes economic and human losses, special requirements from the early stages of design has to be respected. Although the prediction of the aerodynamic phenomena is still a challenging task, engineers focus to design economical bridges with low costs that fulfill the ULS and SLS criteria. Structural modifications, aerodynamic and mechanical measures are considered in order to mitigate the wind induced vibrations. Vortex induced vibration (VIV) is considered as one of the aerodynamic phenomena that can produce fatigue damage accumulation on structural elements and although its effects are analyzed in the framework of the serviceability limit state, its consideration during the design of bridges decks is an undeniable stage. Mitigating the effects of the VIV oscillations can be fulfilled by modifying the shape of the structure since the characteristics of this later affect the vortices direction and can decrease the wind-structure interaction. On the other side, reducing the design cost is an important point to consider. Within this framework comes this paper, which proposes a new strategy to optimize bridges deck while considering the VIV effects.

Structural and material optimization based on thermodynamic principles

Dustin Roman Jantos (*Ruhr-Universität Bochum, Germany*)

17:10

Klaus Hackl (*Ruhr-Universität Bochum, Germany*)

Philipp Junker (*Ruhr-Universität Bochum, Germany*)

In our previous work, we developed a variational approach for topology optimization based on thermodynamic principles, i.e. Hamilton's principle for dissipative processes. The Hamilton's principle yields a closed set of differential equations for a variety of problems in continuum mechanics, which include micro-structural processes described by internal variables (e.g. plasticity, damage modeling, crystallographic transformations, etc.). These internal variables can also be used to describe design variables for an optimization, i.e. structural compliance minimization.

We present a method to derive differential equations for different design variables based on thermodynamic principles: 1) the topology, which is described by a continuous density distribution with penalization of intermediate densities (SIMP), which is regularized by a numerical efficient gradient-enhanced approach; 2) the material distribution of a multi-material model with a tension and a compression affine material, e.g. steel and concrete, in which tension affine material is applied in regions with high tensile stresses and vice versa; 3) the local material orientation of a three-dimensional anisotropic base material, for which we introduce a filtering technique to control the fiber path smoothness for possible manufacturing constraints.

The resulting differential equations yield evolution equations as known from material modeling that can be used as update scheme for an iterative optimization procedure. The explicit updating procedures of the different design variables can be applied in a decoupled scheme and can be combined arbitrarily. Thus, it is also possible to enhance other existing topology optimization approaches (e.g. Optimality Criteria) by including additional design variables, which are updated by evolution equations provided by the presented approach. Numerical results for the topology optimization with tension and compression affine materials, and for the topology and orientation optimization of anisotropic materials will be presented.

Intrinsic formulation of KKT conditions and constraint qualifications on smooth manifolds.

Ronny Bergmann (*Technische Universität Chemnitz, Germany*)

17:30

Roland Herzog (*Technische Universität Chemnitz, Germany*)

We formulate Karush-Kuhn-Tucker (KKT) conditions for equality and inequality constrained optimization problems on smooth manifolds. Under the Guignard constraint qualification, local minimizers are shown to admit Lagrange multipliers. We also investigate other constraint qualifications and provide results parallel to those in Euclidean space. Illustrating numerical examples will be presented.

Composite step method for optimization of equality constrained problems on manifolds

Julian Ortiz (*University of Bayreuth, Germany*)

17:50

Anton Schiela (*University of Bayreuth, Germany*)

In order to exploit the specific structure of certain problems, we generalize the usual constrained optimization setting in which the involved spaces are linear to the setting where the spaces are manifolds. In the vector space setting, the composite step method deals with the problem of feasibility and optimality by splitting the full Lagrange-Newton correction into a normal step and a tangential step, the update iterates are done by adding these corrections to the actual iterate. We extend these ideas to manifolds by using local retractions, which can be thought as local charts of the manifold. First, we pullback the objective and the constraint mappings to linear spaces, there, we compute the normal and tangential corrections and finally the update of the iterates is done even using different retractions defined on the same manifolds. Local superlinear convergence of the algorithm is proven for first order retractions.

We test our method on equilibrium and on optimal control problems in finite elasticity of inextensible Rods. In these problems we optimize over the manifold of kinematically admissible configurations that enforce the inextensibility condition. These examples are test cases for a wider class of mechanical problems in which our method can be used.

Geometry processing problems using the total variation of the normal vector field

Jose Vidal-Nunez (*TU Chemnitz, Germany*)

18:10

Roland Herzog (*TU Chemnitz, Germany*)

Ronny Bergmann (*TU Chemnitz, Germany*)

Stephan Schmidt (*Julius-Maximilians-Universität Würzburg, Germany*)

Marc Herrmann (*Julius-Maximilians-Universität Würzburg, Germany*)

In this talk we present a novel approach to solve geometry processing problems including mesh denoising and surface fairing. As for standard flat images, our goal is to remove noise while preserving shape features such as sharp edges. To this purpose, we first present a continuous version of the total variation of the normal vector.

Then, we model the problem of interest via a quadratic vertex tracking term and a regularizer based on a discrete version of the total variation of the normal field. This discrete regularizer can be seen as an anisotropic variant of its continuous formulation, and it also reduces to a very convenient representation in terms of the geodesic distance on the sphere for piecewise flat (triangulated) surfaces. Finally, we numerically solve the model applying split-Bregman iterations obtaining prominent performance results in the benchmark example of the Fandisk.

S16.04 | MPEC and multilevel optimization

Date: February 21, 2019

08:30-10:30

Room: HS 06

A complementarity-based approach to cardinality-constrained optimization

Alexandra Schwartz (*TU Darmstadt, Germany*)

08:30

Max Bucher (*TU Darmstadt, Germany*)

Sparse optimization problems and optimization problems with cardinality constraints have many applications such as portfolio optimization, subset selection, compressed sensing or learning. In the past, solution approaches have often focused on convex substitutes of the respective problems, e.g. using the l1-norm to induce sparsity. However, recently non convex formulations have gained popularity. In this talk, we give an introduction to a complementarity-based solution approach for cardinality-constrained optimization problems. We focus mostly on tailored optimality conditions as well as a relaxation algorithm. Additionally, we discuss the similarities and differences between classical mathematical programs with complementarity constraints (MPCC) and the complementarity-based reformulation of cardinality-constrained optimization problems.

A multi-leader-multi-follower Nash game with application in gas markets

Daniel Nowak (*TU Darmstadt, Germany, FAU Erlangen-Nürnberg, Germany*)

09:10

Alexandra Schwartz (*TU Darmstadt, Germany*)

Gregor Zöttl (*FAU Erlangen-Nürnberg, Germany*)

We investigate a Multi-Leader-Multi-Follower (MLMF) Nash game, which is inspired by the competition of firms in the Entry-Exit model of a gas market. Here several firms first book a certain capacity for a longer period of time (e.g. a month/year) and then nominate the amount of gas to be sold in several subsequent shorter time periods (e.g. hours/days). The booked amount acts as an upper bound for the nominations. Due to competition in the booking and the nominating step the model results in an MLMF Nash game, where the lower level, i.e. the nominations, is a constrained Cournot-Nash game. One can show the existence and uniqueness of the Nash equilibrium of the lower level. As a first step to approach the Nash equilibrium on the lower level we investigate the behavior of the firms, if the booked capacities are given but fixed. We characterize all possible solutions for each time period and calculate the equilibrium payoffs. As a next step we lift this model to the upper level, where we investigate the behavior of the objective function of every player with respect to the booking variable. We show, that different problems can occur in this step and present ideas, how to deal with these.

The authors thank the Deutsche Forschungsgemeinschaft for their support within the project B09 in the Sonderforschungsbereich / Transregio 154 "Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks".

Multi-leader-single-follower games with unique lower level solution in function space

Jan Becker (*TU Darmstadt, Germany, Graduate School of Excellence Computational Engineering, Germany*)

09:30

Alexandra Schwartz (*TU Darmstadt, Germany, Graduate School of Excellence Computational Engineering, Germany*)

Finite and infinite dimensional Nash equilibrium problems (NEP) are well-known and reasonably well-understood problem classes in game theory. While in a classical NEP we have several players that simultaneously make a decision which influences their own outcome and that of the others, in a multi-leader-follower game (MLFG) the group of players is split into the so-called leaders deciding first and the followers reacting to this.

So far, not that much is known about these hierarchical games, in particular in the function space setting. However, such type of models gained an increasing interest among mathematicians as well as scientist of other fields such as operation research, robotics, computer sciences and economics.

The talk presents an introduction to MLFGs, highlights some difficulties and then focuses on a special subclass: the multi-leader-single-follower game with unique lower level solution.

Under suitable assumptions this can equivalently be written as an equilibrium problem with complementarity constraints (EPCC). By using the special structure of the EPCC as an equilibrium problem where each leader solves a (parametric) mathematical program with complementarity constraints (MPCC) we are able to derive weak and strong stationarity conditions of MLFGs.

Optimal control problems with control complementarity constraints

Christian Clason (*Universität Duisburg-Essen, Germany*)

09:50

Yu Deng (*Technische Universität Bergakademie Freiberg, Germany*)

Patrick Mehlitz (*Brandenburgische Technische Universität Cottbus-Senftenberg, Germany*)

Uwe Prüfert (*Technische Universität Bergakademie Freiberg, Germany*)

A special optimal control problem with complementarity constraints on the control functions is considered. In order to guarantee the existence of optimal solutions for such problems with complementarity constraints, the controls are chosen from a first-order Sobolov space. Some necessary optimality conditions of strong stationary-type are derived by using a standard trick from finite-dimensional MPCC theory. A penalized method based on the Fischer-Burmeister function is constructed and analyzed for solving this problem. Some computational experiments are presented and their solutions are checked by introduced optimality conditions, whether they are strong stationary or not. This talk is based on a joint work with C. Clason, P. Mehlitz and U. Prüfert.

Gradient-based solution algorithms for a class of bilevel optimization and optimal control problems with a non-smooth lower level

Constantin Christof (*TU München, Germany*)

10:10

The aim of this talk is to explore a peculiar regularization effect that occurs in the sensitivity analysis of certain elliptic variational inequalities of the second kind. The effect causes the solution operator of the variational inequality at hand to be continuously Fréchet differentiable although the problem itself contains non-differentiable terms. Our analysis shows in particular that standard gradient based algorithms can be used to solve bilevel optimization and optimal control problems that are governed by elliptic variational inequalities of the considered type - all without regularizing the non-differentiable terms in the lower level problem and without losing desirable properties of the solution as, e.g., sparsity. Our results can, for instance, be used in the optimal control of Casson fluids and in bilevel optimization approaches for parameter learning in total variation image denoising models.

S16.05 | Nonlinear and mixed-integer optimization

Date: February 21, 2019

14:00-16:00

Room: HS 06

A sequential homotopy method for mathematical programming problems

Andreas Potschka (*University Heidelberg, Germany*)

14:00

We consider nonconvex and highly nonlinear mathematical programming problems, whose solutions minimize an objective function over a closed convex subset of a Hilbert space subject to nonlinear equality constraints that map into another Hilbert space. The objective function and constraint function are assumed to be continuously Fréchet-differentiable. This class of problems includes finite dimensional nonlinear programming problems as well as optimization problems with partial differential equations and state/control constraints. We present a novel numerical solution method, which is based on a projected gradient/anti-gradient flow for an augmented Lagrangian on the primal/dual variables. We show that under reasonable assumptions, the nonsmooth flow equations possess uniquely determined global solutions, whose limit points (provided that they exist) are critical, i.e., they satisfy a first-order necessary optimality condition. Under additional mild conditions, a critical point cannot be asymptotically stable if it has an emanating feasible curve along which the objective function decreases. This implies that small perturbations will make the flow escape critical points that are maxima or saddle points. If we apply a projected backward Euler method to the flow, we obtain a semismooth algebraic equation, whose solution can be traced for growing step sizes, e.g., by a continuation method with a local (inexact) semismooth Newton method as a corrector, until a singularity is encountered and the homotopy cannot be extended further. Moreover, the projected backward Euler equations admit an interpretation as necessary optimality conditions of a proximal-type regularization of the original problem. The prox-problems have favorable properties, which guarantee that the prox-problems have uniquely determined primal/dual solutions if the Euler step size is sufficiently small and the augmented Lagrangian parameter is sufficiently large. The prox-problems morph into the original problem when taking the step size to infinity, which allows the following active-set-type sequential homotopy method: From the current iterate, compute a projected backward Euler step by applying either local (inexact) semismooth Newton iterations on the step equations or local (inexact) SQP-type (sequential quadratic programming) methods on the prox-problems. If the homotopy cannot be continued much further, take the current result as a starting point for the next projected backward Euler step. If we can drive the step size all the way to infinity, we can transition to fast local convergence. We can interpret this sequential homotopy method as extensions to several well-known but seemingly unrelated optimization methods: A general globalization method for local inexact semismooth Newton methods and local inexact SQP-type methods, a proximal point algorithm for problems with explicit constraints, and an implicit version of the Arrow–Hurwicz gradient method for convex problems dating back to the 1950s extended to nonconvex problems. We close the talk with numerical results on large-scale highly nonlinear and badly conditioned mathematical programming problems and an outlook on future directions of research.

A hybrid semismooth-/quasi-Newton method (not only) for structured nonsmooth optimization

Florian Mannel (*University of Graz, Austria*)

14:40

Armin Rund (*University of Graz, Austria*)

We present an algorithm for the efficient solution of structured nonsmooth operator equations in Banach spaces. Here, the term structured indicates that we consider equations which are composed of a smooth and a semismooth mapping. Equations of this type occur, for instance, as optimality conditions of structured nonsmooth optimization problems such as LASSO in machine learning.

The novel algorithm combines a semismooth Newton method with a quasi-Newton method. This hybrid approach retains the local superlinear convergence of both these methods under standard assumptions. Since it is known that quasi-Newton methods alone can generally not achieve superlinear convergence in semismooth settings, this is rather satisfying from a theoretical point of view.

The most striking feature of the new method, however, is its numerical performance. On nonsmooth PDE-constrained optimal control problems it is significantly faster than semismooth Newton methods, and these speedups persist when globalization techniques are added. Most notably, the hybrid approach can be embedded in a matrix-free limited-memory truncated trust-region framework to efficiently solve nonconvex and nonsmooth large-scale real-world optimization problems, as we will demonstrate by means of an example from magnetic resonance imaging. In this challenging environment it dramatically outperforms semismooth Newton methods, sometimes by a factor of fifty and more.

All of these topics are addressed in the talk.

An approximation scheme for distributionally robust nonlinear optimization

Johannes Milz (*Technical University of Munich, Germany*)

15:00

Michael Ulbrich (*Technical University of Munich, Germany*)

We consider distributionally robust optimization problems (DROPs) with nonlinear and non-concave dependence on uncertain parameters. To obtain tractable and accurate lower-level optimization problems, we define ambiguity sets through moment constraints and, moreover, we approximate nonlinear functions using quadratic expansions w.r.t. parameters resulting in lower-level problems defined by trust-region problems and semidefinite programs. Subsequently, we construct smoothing functions for the approximate optimal value functions, which can efficiently be evaluated, and show that gradient consistency holds. We apply a homotopy method to smooth DROPs dynamically decreasing smoothing parameters and establish its convergence to stationary points of the approximate DROP under mild assumptions. We provide illustrative numerical examples showing the efficiency of our approach.

Penalty formulations for mixed integer and PDE constrained optimization problems

Dominik Garmatter (*Chemnitz University of Technology, Germany*)

15:20

Martin Stoll (*Chemnitz University of Technology, Germany*)

This talk shall deal with optimal control problems with a partial differential equation (PDE) as constraint and additional integer constraints for the control, or in short mixed integer PDE constrained optimization (MIPDECO) problems. In order to satisfy the integrality constraints, mixed integer optimizations problems are usually solved by Branch-and-Bound (BnB) solvers. These methods find the globally optimal solution by searching the combinatorial tree provided by the integrality constraints in a clever and efficient way. The obvious drawback of these BnB methods in a PDE constrained framework is, that the combinatorial complexity provided by a discretization of a PDE constraint can quickly become too challenging for BnB solvers up to the point where they can not find a satisfactory solution in finite time.

As a remedy to this situation, we will investigate various penalty formulations that replace the integrality constraint in the MIPDECO problem by a suitable penalty term in the objective

function. Instead of dealing with integrality constraints, one now has to choose the penalty parameter in such a way that an integer solution is obtained that still fits the desired state. In order to do so, we will repeatedly solve the optimization problem for an increasing sequence of penalty parameters until an integer (or near-integer) solution is found. Based on two penalty formulations, we will present corresponding algorithms and, for a numerical test example, compare these algorithms with two basic rounding strategies and a BnB-routine.

Multi-dimensional sum-up rounding

Paul Manns (*TU Braunschweig, Germany*)

15:40

Christian Kirches (*TU Braunschweig, Germany*)

Mixed-Integer Optimal Control Problems (MIOCPs) that are constrained by time-dependent differential equations can be reformulated by means of partial outer convexification which introduces switching functions for the different realizations of a discrete-valued control variable. The switching functions are 0,1-valued and a natural relaxation arises by allowing them to take values in $[0,1]$.

Sum-Up Rounding algorithms approximate feasible switching functions of the relaxed problem with 0,1-valued ones that are feasible or feasible up to an arbitrarily small $\delta > 0$, depending on the constraints. The key insight is that the approximants converge in a weak topology when the coarseness of the rounding grid is driven to zero. Consequently, the associated state vector sequence converges in norm provided the underlying differential equation features sufficient regularity properties. This in turn enables us to employ continuity properties of constraint or objective functions w.r.t. to the state vector.

We show that the above-described approximation properties can be transferred to MIOCPs with discrete-valued variables being distributed in more than one dimension. For this purpose, we take advantage of an appropriate grid refinement strategy that is coupled with a deliberate ordering of the grid cells during the refinements. We provide a sufficient condition for such ordering strategies and demonstrate that it is satisfied by the approximants of space-filling curves. This allows us to deduce a norm convergence result for the state vector of elliptic PDE systems. Furthermore, we provide computational results illustrating the applicability of the theoretical framework and gives hints to its limitations.

S16.06 | Nonsmooth optimization I

Date: February 21, 2019

17:40-18:40

Room: HS 06

On a new linearization approach for nonsmooth optimization

Andrea Walther (*Universität Paderborn, Germany*)

17:40

Andreas Griewank (*Yachaytech, Ecuador*)

For finite dimensional problems that are unconstrained and piecewise smooth the optimization based on successive abs-linearisation is well analysed yielding for example linear or even quadratic convergence under reasonable assumptions on the function to be optimised. In this talk we discuss the extension of this approach to the more general class of nonsmooth but still Lipschitz continuous functions covering also the Euclidean norm. For this purpose, we introduce the so-called clipped root linearisation and present first numerical results.

On the relation between MPECs and optimization problems in abs-normal form

Lisa Christine Hegerhorst-Schultchen (*Leibniz Universität Hannover, Germany*) 18:00

Christian Kirches (*Technische Universität Carolo-Wilhelmina zu Braunschweig*)

Marc Christian Steinbach (*Leibniz Universität Hannover, Germany*)

Nonsmoothness arises in many practical optimization problems. Models using the absolute value, the maximum or minimum function are prominent examples. These can be formulated as (unconstrained) optimization problems in abs-normal form. Another example are complementarity conditions which lead to the problem class of MPECs.

In this talk we show that the class of unconstrained optimization in abs-normal form is a subclass of the class of MPECs and that the class of constrained optimization in abs-normal form is equivalent to the class of MPECs. Moreover, we compare constraint qualifications and stationarity concepts of these problem classes and observe close relations between them.

On the hierarchical structure of Pareto critical sets in multiobjective optimization

Bennet Gebken (*Paderborn University, Germany*) 18:20

Sebastian Peitz (*Paderborn University, Germany*)

Michael Dellnitz (*Paderborn University, Germany*)

Given an unconstrained multiobjective optimization problem (MOP) with n variables and k differentiable objectives, a necessary condition for (local) Pareto optimality at some point x is the non-existence of a common descent direction of all objective functions. Such x are called Pareto critical and they form a set P called the Pareto critical set. The Pareto critical set can be equivalently described using the Karush-Kuhn-Tucker (KKT) conditions: x is Pareto critical if and only if there is a convex combination of the gradients of the objective functions in x that is zero (cf. Miettinen (1998)).

If all objective functions are smooth, convex and k is not larger than n , then P is diffeomorphic to a $(k - 1)$ -dimensional simplex, so its structure is well understood (cf. Smale (1973)). To be precise, each of its facets is given by a Pareto critical set of an MOP that consists of $k - 1$ objective functions of the original MOP. There are also results about the structure for the general case showing that generically, P is a stratified set (cf. de Melo (1976)). Roughly speaking, this means that it is a manifold with boundary and corners. First results about its boundary indicate that it is still given by subproblems with fewer objective functions (cf. Lovison and Pecci (2014) and Peitz (2017)).

In this talk we show that the boundary of the Pareto critical set P of an unconstrained and differentiable MOP indeed consists of Pareto critical points of subproblems that only consider a subset of the set of original objective functions. This result does not only give a better understanding of the theoretical properties of P , but can also be directly used in numerical methods: If P is completely described by its boundary (e.g., if we have more objective functions than variables), it can be computed by first computing the boundary and then "filling out" certain connected components in the boundary structure. Since generically, the boundary of P has a lower dimension than P itself, this approach can drastically reduce the time needed to compute the Pareto critical set, and therefore, the Pareto set.

S16.07 | Nonsmooth optimization II

Date: February 22, 2019

08:30-10:30

Room: HS 06

Why under certain conditions one-dimensional search for the optimum of a function is really Fibonaccian.

Herbert Niessner (*NiMa, Switzerland*)

08:30

Consider searches for the optimum of a function along a line. Most descriptions of the Fibonacci search method (e.g. Kiefer 1953, Kowalik-Osborne 1968, Pierre 1969) start using Fibonacci numbers at the very beginning. It will be shown why this numbers come into play. Corresponding formulas and those for the golden section search are completely derived.

Theory and numerical practice for optimization problems involving l^p functionals, with p in $[0,1)$

Daria Ghilli (*University of Graz, Austria*)

08:50

Karl Kunisch (*University of Graz, Austria*)

Nonsmooth nonconvex optimization problems involving the l^p quasi-norm, p in $[0,1)$, of a linear map are considered. A monotonically convergent scheme for a regularized version of the original problem is developed and necessary optimality conditions for the original problem in the form of a complementary system amenable for computation are given. Then an algorithm for solving the above mentioned necessary optimality conditions is proposed. It is based on a combination of the monotone scheme and a primal-dual active set strategy. The performance of the two schemes is studied and compared to other existing algorithms by means of a series of numerical tests in different cases, including optimal control problems, fracture mechanics and microscopy image reconstruction.

First-order methods and model splitting techniques for non-convex non-smooth optimization

Tuomo Valkonen (*Escuela Politécnica Nacional, Ecuador, University of Helsinki, Finland*)

09:10

Christian Clason (*University Duisburg-Essen, Germany*)

Stanislav Mazurenko (*University of Liverpool, UK*)

Convex optimisation problems can frequently be solved more efficiently by converting their original, primal, form into a dual form, or, better yet, a saddle-point form; first-order algorithms for the latter including the Chambolle-Pock method or primal-dual proximal splitting (PDPS), as well as the classical ADMM and its preconditioned variants. Until recently, non-convex problems were most commonly solved by second-order methods in their primal form. In this talk, we present ways to reformulate non-convex non-smooth problems as general saddle point problems that split into a convex non-smooth part, and a non-convex smooth part. We then study extensions of the PDPS to such problems, illustrating the performance on practical inverse problems.

A primal-dual algorithm for risk minimization

Thomas M. Surowiec (*Philipps-Universität Marburg, Germany*)
Drew P. Kouri (*Sandia National Laboratories, USA*)

09:30

We present an algorithm for the efficient solution of risk-averse optimization problems. The setting is broad enough to include finite and infinite dimensional optimization problems arising, for example, in PDE-constrained optimization under uncertainty. As many popular risk models such as coherent risk measures are nonsmooth, special care needs to be taken to develop viable algorithmic approaches. To address the many challenges arising in numerical approximation and solution, we propose a new primal-dual algorithm for solving large-scale nonsmooth risk-averse optimization problems. The algorithm combines ideas from the classical method of multipliers with a recently developed variational regularization technique for convex risk measures. The resulting algorithm solves a sequence of smooth optimization problems using existing derivative-based approaches. We prove convergence of the algorithm for inexact subproblem solves and nonconvex objectives. The performance is illustrated with numerical examples.

Random function iterations for stochastic fixed point problems

Neal Hermer (*Universität Göttingen, Germany*)
Russell Luke (*Universität Göttingen, Germany*)
Anja Sturm (*Universität Göttingen, Germany*)

09:50

We study the convergence of iterated random functions for stochastic fixed point iterations in the inconsistent case. What distinguishes inconsistent fixed point iterations from their consistent counterpart studied in Hermer, Luke and Sturm [Numer. Funct. Anal. Optimiz., 2018] (to appear) is that the mappings need not have (almost surely) common fixed points. Convergence of such random function iterations is most appropriately defined in terms of weak convergence of the distributions of the iterates. Existence of invariant measures is established for continuous (Feller) Markov operators associated with fixed point iterations inspired by first-order proximal methods in optimization (e.g. the Douglas-Rachford, and proximal-point algorithms) for several examples. Convergence of sequences of iterated random functions is established for ergodic nonexpansive mappings and nonergodic sequences under the assumption that the mappings are averaged.

S17 | Applied and numerical linear algebra

Organiser: Oliver Rheinbach (*Technische Universität Bergakademie Freiberg, Germany*)
Alexander Heinlein (*University of Cologne, Germany*)

S17.01 | Applied and numerical linear algebra

Date: February 19, 2019
Room: Elise-Richter HS

08:30-10:30

Model reduction techniques for port-Hamiltonian differential-algebraic systems

Sarah-Alexa Hauschild (*Universität Trier, Germany*) 08:30
Nicole Marheineke (*Universität Trier, Germany*)
Volker Mehrmann (*Technische Universität Berlin, Germany*)

Port-based network modelling of large multi-physics systems leads naturally to their formulation as port-Hamiltonian differential-algebraic systems. The port-Hamiltonian structure is closely related to the properties of the system, e.g., passivity. Furthermore, the state space dimension of such systems can easily become very large, as they arise from electrical circuits, multi-body systems or semi-discretization of partial differential equations. Thus, there is an immediate need for structure-preserving model reduction methods. While reducing the order of differential-algebraic equations, keeping the algebraic constraints unchanged is important. Otherwise, properties like stability can be lost. Thus, the aim of this paper is to decouple the underlying ordinary differential equation and the algebraic constraints in a structure-preserving manner and to adapt model reduction methods for ordinary port-Hamiltonian systems to port-Hamiltonian differential-algebraic systems, such that the structure and the algebraic constraints are preserved.

Parametric model order reduction based on H2xL2 optimality conditions

Manuela Hund (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*) 08:50
Petar Mlinarić (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

We consider parametric linear time-invariant systems. These systems arise in various mathematical and physical processes, where the parameters describe, e.g., geometrical or physical constants. Often, the dimension of these systems is too large to efficiently simulate them for many parameter values. Thus, our aim is to compute reduced-order models (ROM) that are much faster to evaluate and have the same input-output behavior.

One way to achieve this in the non-parametric setting is H2 optimal model order reduction. Here, David A. Wilson derived necessary optimality conditions, which are given as a set of coupled matrix equations.

We extend this idea to the parametric case. Therefore we also have to take the optimality with respect to the parameters into account. A possible tool to handle this is the L2 norm. The only assumption we make on the ROM is an affine decomposition of its matrices. This leads to integral matrix equations as H2 x L2 necessary optimality conditions. In case the full-order matrices are

affine decomposable, this approach can preserve the given structure. Otherwise if the matrices of the original system are unstructured, this procedure obtains a ROM with structured matrices. In our contribution, we will show how these Wilson-type optimality conditions can be handled to obtain a ROM. Therefore, we will present an algorithm based on the gradient descent method and show first numerical results.

On the application of a greedy reduced basis scheme to the multi-frequency solution of acoustic boundary element equations

Christopher Jelich (*Technical University of Munich, Germany*)

09:10

Suhaib Koji Baydoun (*Technical University of Munich, Germany*)

Steffen Marburg (*Technical University of Munich, Germany*)

In this work, a greedy reduced basis scheme for the multi-frequency solution of linear time-harmonic acoustic problems is investigated. This scheme allows to express the approximate solution within a frequency range of interest as a linear combination of a few basis vectors. These basis vectors are given by the solutions of the underlying frequency dependent linear system at iteratively chosen frequency samples. In each step of the algorithm, the next basis vector is evaluated at a frequency point for which the solution is worst approximated by the current reduced basis. In order to approximate the solution between the frequency points as well as to compute a posteriori error estimations, a least square solver is used. Further, the boundary element method is used for discretizing the underlying Helmholtz problem and an iterative solver is applied for the solution of the high-fidelity system. Seeking to solve medium to large-scale problems, a data sparse representation of the system matrix in the form of an H2-matrix is introduced. This reduces both the memory requirements of the scheme as well as the computational effort of the matrix-vector products. The performance of the proposed scheme is shown based on interior and exterior acoustic problems. Comparisons to conventional multi-frequency strategies verify the efficiency of the method.

Linear algebra properties of dissipative Hamiltonian systems

Volker Mehrmann (*TU Berlin, Germany*)

09:30

Christian Mehl (*TU Berlin, Germany*)

Michal Wojtylak (*Uniwersytet Jagiellonski, Poland*)

Dissipative Hamiltonian systems arise in a large number of applications. For the linear constant coefficient case surprising spectral properties arise directly from the structure. It is shown that all eigenvalues are in the closed left half plane, those on the imaginary axis are semisimple except for the eigenvalue zero and the eigenvalue infinity which can have Jordan blocks of size at most two. Also the left and right minimal indices are restricted. These properties also lead to strong restrictions for stability radii and the associated perturbation analysis.

Topological analysis of FMUs in liquid flow networks

Ann-Kristin Baum (*RICAM, Austria, MathConsult, Austria*)

09:50

Michael Kolmbauer (*MathConsult, Austria*)

Günter Offner (*AVL List GmbH, Austria*)

We consider the analysis of multi-physics dynamical systems stemming from automated modeling processes in system simulation software. Today's system modeling software typically offers a wide range of basic physical components from several domains, which can be assembled to customized physical networks simply by drag and drop. The governing equations are derived by

representing the network as a linear graph whose edges and nodes correspond to the basic physical components. Combining the connection structure of the graph with the physical equations of the components, the physical network is modeled as Differential-Algebraic Equations (DAE). Using algebraic graph and DAE theory, the solvability of the mathematical model is analyzed and translated as conditions on the network structure and properties of its elements. To control these networks or to connect them to the environment, boundary conditions are present, allowing to incorporate external or user defined components. In many cases, these external components are given by black-box models. Recently e.g. the Functional Mock-up Unit (FMU) has been established as a standardized structured interface, giving the input-output relation as differential state and algebraic output equation. The explicit symbolic representation of the equations is unknown, however, the entry pattern of the Jacobians of these equations is given. Incorporating these types of black-box components into physical networks may thus drastically affect its physical validity and solvability. Based on our previous work regarding the solvability of liquid flow networks, we present non-trivial conditions on the network structure, its elements and the coupled FMUs that allow to preserve the physical validity as well as the solvability of the physical network. Exploiting graph theoretical and DAE concepts, we identify those boundary conditions that may be replaced by FMUs, specify what kind of FMUs may be included regarding their input-output-relation and by what type of physical element they are allowed to be connected to the network. We specify the feasible set of initial conditions and construct a surrogate model allowing for a robust and efficient simulation of the network. Keeping a close connection between the topology and the equations of the network, we are able to translate the non-trivial solvability conditions of the model as easy-to-check graph theoretical conditions on the network. Having typically problems of the size 10^3 unknowns, this is particular important.

Kemeny's constant and Braess' paradox

Stephen Kirkland (*University of Manitoba, Canada*)

10:10

For a Markov chain with an irreducible transition matrix, Kemeny's constant measures the expected number of steps for the Markov chain to transit from a randomly chosen initial state to a randomly chosen destination state. In particular, if Kemeny's constant is small then we can think of the Markov chain as having good mixing properties. For the special case of a random walk on an undirected graph, Kemeny's constant thus provides an overall measure of the efficiency of the corresponding network. In this talk, we focus on graphs for which adding a new edge has the counterintuitive effect of increasing Kemeny's constant. This surprising effect mirrors Braess' paradox for vehicle traffic networks, whereby opening a new route can actually increase travel times.

S17.02 | Applied and numerical linear algebra

Date: February 19, 2019

16:30-18:30

Room: Elise-Richter HS

Computational homogenization in EXASTEEL

Axel Klawonn (*Universität zu Köln, Germany*)

16:30

Stephan Köhler (*Technische Universität Bergakademie Freiberg, Germany*)

Martin Lanser (*Universität zu Köln, Germany*)

Oliver Rheinbach (*Technische Universität Bergakademie Freiberg, Germany*)

In the EXASTEEL project, computational homogenization using the FE^2 approach is combined with fast domain decomposition solvers for simulations with million-way parallelism. Recent results are discussed using structured as well as unstructured meshes for the representative volume elements (RVEs).

EXASTEEL: developments in nonlinear and linear domain decomposition methods

Martin Lanser (*University of Cologne, Germany*)

16:50

Axel Klawonn (*University of Cologne, Germany*)

Oliver Rheinbach (*TU Bergakademie Freiberg, Germany*)

In the project "EXASTEEL - Bridging Scales for Multiphase Steels" (part of the German priority program SPPEXA) we are concerned with the simulation of modern dual-phase steels. A virtual laboratory is developed to simulate the Nakajima test, to compute FLCs (Forming Limit Curves), and to predict the formability and ductility of certain steels. These properties are strongly influenced by the microscopic structure of the material, which is resolved in our computations by the scale bridging and homogenization approach FE². We implemented the highly scalable software package FE2TI, which combines FE² and highly scalable nonlinear and nonlinear DD (domain decomposition) implicit solvers, which are used on the microscopic level and themselves can efficiently scale up to the largest computers. In this talk, the developments and implementations of different nonlinear and linear domain decomposition methods achieved and used in EXASTEEL are described and compared. Weak scalability up to hundreds of thousands of compute cores is shown.

FROSch - a parallel implementation of the GDSW domain decomposition preconditioner in Trilinos

Alexander Heinlein (*Universität zu Köln, Germany*)

17:10

Axel Klawonn (*Universität zu Köln, Germany*)

Oliver Rheinbach (*Technische Universität Bergakademie Freiberg, Germany*)

The FROSch (Fast and Robust Overlapping Schwarz) library, a parallel implementation of the GDSW (Generalized Dryja Smith Widlund) preconditioner, has recently been integrated into Trilinos as part of the package ShyLU. The GDSW preconditioner has been introduced by Dohrmann, Klawonn, and Widlund in 2008 and is a two-level overlapping Schwarz preconditioner with an energy-minimizing coarse space that is inspired by non-overlapping domain decomposition methods, such as FETI-DP and BDDC methods. It is robust for a wide class of problems, e.g., solid or fluid mechanics, and can be constructed in an algebraic way. In particular, the coarse space can be constructed from the fully assembled matrix without an additional coarse triangulation, even for irregular subdomains. However, the preconditioner can benefit from additional information about the problem.

This talk gives an overview of the FROSch code, its features, and user-interface and shows the parallel scalability and robustness of the solver for several problems. In particular, FROSch is applied to scalar elliptic problems, linear elasticity, and nonlinear elasticity in fluid-structure interaction applications and as a monolithic preconditioner for saddle-point problems. Parallel scalability of the code is shown up to a maximum of 64K cores using a direct coarse solver on one core.

A three-level GDSW overlapping Schwarz preconditioner

Alexander Heinlein (*Universität zu Köln, Germany*)

17:30

Axel Klawonn (*Universität zu Köln, Germany*)

Oliver Rheinbach (*Technische Universität Freiberg, Germany*)

Friederike Röver (*Technische Universität Freiberg, Germany*)

The GDSW preconditioner is a two-level overlapping Schwarz preconditioner with an energy-minimizing coarse space, which can be constructed algebraically from the assembled matrix. To improve the weak parallel scalability of the two-level method a three-level extension has been introduced. Here, the GDSW preconditioner is applied recursively to the coarse problem. Numerical results, obtained for a parallel implementation using the Trilinos software library, in two and three dimensions are presented. A further improvement of the scalability can be obtained by reducing the dimension of the coarse space. Results for the three- and two-level method applying a reduced coarse space are also presented. Regarding the size of the coarse problem the new methods can be expected to scale when the classical method will be out of memory.

A time adaptive multirate Dirichlet-Neumann waveform relaxation method for heterogeneous coupled heat equations

Azahar Monge (*University of Deusto, Spain*)

17:50

Philipp Birken (*Lund University, Sweden*)

The efficient simulation of thermal interaction between fluids and structures is crucial in the design of many industrial products, e.g. thermal anti-icing systems of airplanes, gas quenching, which is an industrial heat treatment of metal workpieces or the cooling of rocket thrust chambers. Unsteady thermal fluid structure interaction is modelled using two partial differential equations describing a fluid and a structure which are coupled at an interface. The standard algorithm to find solutions of the coupled problem is the Dirichlet-Neumann iteration, where the PDEs are solved separately using Dirichlet-, respectively Neumann boundary with data given from the solution of the other problem. Previous analysis and numerical experiments show that this iteration is fast for the thermal coupling of air and steel [2]. This method has the main disadvantage that both fields are solved with a common time resolution. Using instead a time adaptive multirate scheme would be more efficient.

In view of this, we present here a high order, time adaptive, multirate numerical method for two heterogeneous coupled heat equations. We use the Dirichlet-Neumann waveform relaxation (DNWR) method which is a variant of WR methods based on the classical Dirichlet-Neumann iteration [1]. When choosing the relaxation parameter right, the iterative DNWR becomes a direct solver. We present an analysis of the DNWR algorithm that shows that the optimal relaxation parameter is highly dependent on the material coefficients. We performed a similar analysis for the Neumann-Neumann waveform relaxation (NNWR) algorithm [3]. In order to get an adaptive multirate scheme, we use possibly different adaptive temporal discretization methods on the two subdomains. Furthermore, two time integration alternatives are presented, the implicit Euler method and a second order singly diagonally implicit Runge-Kutta method (SDIRK2).

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Asynchronous time integration in structural mechanics

Andreas S. Seibold (*TU München, Germany*)

18:10

Daniel Jean Rixen (*TU München, Germany*)

When decomposing structural dynamics simulations it might become necessary to refine several substructures' meshes due to physics, for example local damaging. The same can be done with time step sizes resulting in so called asynchronous or multirate time integration techniques. For such a purpose and to couple different integration schemes, resulting in heterogeneous time integration, interpolation-methods between coarse time-scales have been developed to achieve the solves on finer time-scales [2, 4]. Asynchronous time-steps might lead to bad load balancing in parallel computations though. Therefore the space-time domain can not only be decomposed in space, but in time as well [1]. This can be very useful, if one has more computing cores available than is suitable for domain-decomposition in space. In accordance with the FETI-method, Lagrange-multipliers have been used to couple those time-domains [1, 3] and by introducing a third interface-field, this method has been further extended, allowing greater flexibility in the chosen time-steps and integration-schemes and coupling it with non-conforming mesh-interfaces [5]. Since we want to extend our FETI-framework with such an asynchronous time-integrator, a Lagrange-multiplier-based framework should suit us best. Furthermore the time step sizes should be changeable during the simulation process in a flexible manner, for example due to local cracks in substructures. Hence we further investigate these integration methods. Especially energy conservation in nonlinear dynamics and the combination with a FETI-solver are of particular interest.

References

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S17.03 | Applied and numerical linear algebra

Date: February 20, 2019

08:30-09:30

Room: Elise-Richter HS

An algebraic multigrid method for linear elasticity

Joachim Schöberl (*TU Wien, Austria*)

08:30

Lukas Gerhard Kogler (*TU Wien, Austria*)

In this talk we present a new variation of Smoothed Aggregation AMG for linearized elasticity. The method directly incorporates rigid body modes into the coarse spaces, which feature both translational and rotational degrees of freedom. Coarsening and smoothing are both based on a replacement matrix which induces an equivalent norm to the energy norm. It is, however, of a simpler structure than the system matrix, as it only consists of edge contributions which are computed from element matrices during the assembly loop and can be kept unassembled. This gives us a simple way to smooth out coarse basis functions while preserving rigid body modes.

Local Fourier analysis of multigrid smoothers for the Stokes problem

Lisa Claus (*Bergische Universität Wuppertal, Germany*)

08:50

Matthias Bolten (*Bergische Universität Wuppertal, Germany*)

Multigrid methods are efficient iterative solvers for the solution of partial differential equations (PDEs). The efficiency of multigrid methods is due to the combination of suitable smoothers with a coarse grid correction. As one of the two key ingredients, smoothers have a significant impact on the performance of multigrid solvers. Most of the literature on smoothers in multigrid methods is concerned with scalar PDEs, only. Systems are considered less often. In this talk, we compare the commonly used Vanka smoother with a nonoverlapping variant of the Vanka smoother. While the latter is computationally cheaper, the convergence depends much more on the implementation than that of the overlapping method. A Local Fourier Analysis and a general comparison including the computational cost and the convergence properties of the two different methods, for finite differences on staggered grids, will be presented.

Parallel block-selective algebraic multigrid in foam-extend

Tessa Uroic (*Faculty of Mechanical Engineering and Naval Architecture, Croatia*)

09:10

Hrvoje Jasak (*Faculty of Mechanical Engineering and Naval Architecture, Croatia*)

Multigrid methods were originally created for systems of discretised elliptic PDEs but were later expanded and have proven to be efficient for general types of PDEs. Multigrid methods exploit the fact that the point-fixed methods (Jacobi, Gauss-Seidel) tend to quickly reduce the high frequency solution errors, i.e. the errors whose direction corresponds to the largest eigenvalues of the matrix. However, the low frequency errors remain and this is why the performance (convergence) of the fixed-point methods deteriorates. To solve this issue, multigrid methods construct a hierarchy of grids by coarsening the initial grid. The low frequency errors on the finer grid become high frequency errors on the coarser grid and the fixed-point algorithms are able to efficiently reduce these errors. The correction obtained on the coarser grid is then transferred back to the finer grid. Algebraic multigrid methods operate on matrix coefficients directly and do not need a computational grid. We have implemented an algebraic multigrid method in OpenFOAM, an open-source toolbox for Computational Fluid Dynamics based on the Finite Volume Method. The algorithm closely follows the work by K. Stueben and T. Clees and is used to solve the implicitly coupled pressure-velocity system. The numerical discretisation of the linearised equations produces a sparse point-ordered block matrix. To apply the scalar matrix algorithm, a primary matrix is defined and used in the coarsening process. Since the algorithm is used to solve very large systems, a parallel version was developed, without using the subdomain blocking technique as suggested by the original authors. In this work, we present the parallelisation strategy and performance of the block-selective algebraic multigrid for incompressible turbulent flow cases. We will also review the findings on the optimal choice of smoother, multigrid cycle and other settings.

S17.04 | Applied and numerical linear algebra

Date: February 20, 2019

14:00-16:00

Room: Elise-Richter HS

Constructing algebraic preconditioners from domain decomposition

Alexander Heinlein (*Universität zu Köln, Germany*)

14:00

Jascha Knepper (*Universität zu Köln, Germany*)

Axel Klawonn (*Universität zu Köln, Germany*)

Oliver Rheinbach (*TU Freiberg, Germany*)

The GDSW algorithm is a parallel two-level overlapping Schwarz preconditioner for sparse linear systems which can be constructed algebraically from the assembled matrix. The adaptive GDSW algorithm enhances the coarse problem of the GDSW algorithm by eigenvectors computed from local eigenvalue problems. The resulting method fulfills a condition number bound depending only a used-defined threshold. The local eigenvalue problems can be constructed from local subdomain matrices.

On a scalable, highly robust domain decomposition method with dynamic load balancing

Martin Kühn (*Cerfacs, Toulouse, France, University of Cologne, Germany*)

14:20

Axel Klawonn (*University of Cologne, Germany*)

Oliver Rheinbach (*TU Bergakademie Freiberg, Germany*)

Domain decomposition methods such as FETI-DP (Finite Element Tearing and Interconnecting - Dual Primal) and BDDC (Balancing Domain Decomposition by Constraints) are highly scalable parallel solvers for large sparse systems obtained from the discretization of partial differential equations (PDEs).

However, the convergence behavior of FETI-DP and BDDC methods with a standard coarse space highly depends on the parameters of the underlying PDE. The convergence rate of both methods can deteriorate significantly if composite materials are considered. In such cases, problem-dependent (or adaptive) coarse spaces offer a remedy. In adaptive methods, difficulties arisen from highly heterogeneous materials are detected automatically by solving local generalized eigenvalue problems and an adaptive coarse space is set up. These methods are thus characterized by great robustness.

Though, for an efficient parallel implementation, different issues such as load imbalances and the solution of unnecessary eigenvalue problems have to be avoided and the eigenvalue solver has to be optimized to reduce the computational overhead in the set up phase. We will present details of the set up of the adaptive method to implement the coarse space enrichment efficiently in a parallel context.

We will present weak and strong scaling results to show the good parallel scalability of our method.

Machine learning in adaptive domain decomposition methods - predicting the geometric location of constraints

Alexander Heinlein (*Universität zu Köln, Germany*)

14:40

Axel Klawonn (*Universität zu Köln, Germany*)

Martin Lanser (*Universität zu Köln, Germany*)

Janine Weber (*Universität zu Köln, Germany*)

The convergence rate of domain decomposition methods is generally determined by the eigenvalues of the preconditioned system. For second-order elliptic partial differential equations, coefficient discontinuities with a large contrast can lead to a deterioration of the convergence rate. A remedy can be obtained by enhancing the coarse space with elements, which are often called constraints, that are computed by solving small eigenvalue problems on portions of the interface of the domain decomposition, i.e., edges in two dimensions or faces and edges in three dimensions. In the present work, without restriction of generality, the focus is on two dimensions. In general, it is difficult to predict where these constraints have to be computed, i.e., on which edges. Here, a machine learning based strategy using neural networks is suggested to predict the geometric location of these edges in a preprocessing step. This reduces the number of eigenvalue problems that have to be solved during the iteration. Numerical experiments for model problems and realistic microsections using regular decompositions as well as those from graph partitioners are provided, showing very promising results.

Logistic regression for potential modeling

Samuel Kost (*Technische Universität Freiberg, Germany*) 15:00
Helmut Schaben (*Technische Universität Freiberg, Germany*)
Oliver Rheinbach (*Technische Universität Freiberg, Germany*)
Michael Eiermann (*Technische Universität Freiberg, Germany*)

Regression or regression-like models are often employed in potential modeling either based on 2D map images or 3D geomodels both in raster mode or based on spatial point processes. Since prediction of a target event is the ultimate objective, machine learning techniques like artificial neural networks are often employed and give decent results in prediction. However they provide almost no insight into the problem about importance of covariables or even necessity of those. We propose a series of logistic regression models to create a decent final model for prediction. The use of truncated Newton methods enables the procedure to process in reasonable time.

Large scale non-autonomous differential Riccati equations

Björn Baran (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*) 15:20
Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Our motivating example is the feedback stabilization of a two-dimensional two-phase Stefan problem. After linearization and discretization, it results in a non-autonomous differential Riccati equation (DRE) with differential-algebraic structure. The Stefan problem can model solidification and melting of pure materials. This model gets its name from the purely algebraic Stefan condition which describes the coupling between the temperature of the material and its melting process. Even more differential-algebraic structure is introduced through the coupling of the Stefan problem with the Navier–Stokes equations. The two phases in the domain evolve, which causes all coefficients of the resulting DRE to be time-varying. In the literature there exist several methods to numerically solve DREs, e.g. backward differentiation formulas (BDF), Rosenbrock methods, and splitting methods. These methods are well studied for autonomous DREs. However, several difficulties arise when they are adapted to solve non-autonomous DREs, like time dependent terms that vanish only in the autonomous case and larger memory costs for the time-varying data. We present several techniques to tackle the difficulties and implement a non-autonomous BDF method.

Fast computation of optimal damping parameters for linear vibrational systems

Ivan Slapničar (*University of Split, Croatia*)

15:40

Nevena Jakovčević Stor (*University of Split, Croatia*)

Zoran Tomljanović (*University of Osijek, Croatia*)

We formulate the quadratic eigenvalue problem underlying the mathematical model of a linear vibrational system as an eigenvalue problem of a diagonal-plus-rank-one matrix A . The eigenvector matrix of A has Cauchy-like structure. We compute the trace of the solution of the Lyapunov equation $AX + XA^* = -GG^*$, where G is a low-rank matrix which depends on the damped eigenfrequencies, using fast multiplication of linked Cauchy-like matrices. The trace is computed in $O(k^2n^2)$ operations, where $k \ll n$ is the number of dampers. Hence, the subsequent optimization is order of magnitude faster than in the standard approach.

S17.05 | Applied and numerical linear algebra

Date: February 20, 2019

16:30-18:30

Room: Elise-Richter HS

Numerical behavior of GMRES for singular systems

Miroslav Rozložnik (*Czech Academy of Sciences, Czech Republic*)

16:30

Keiichi Morikuni (*University of Tsukuba, Japan*)

In this contribution, we study the numerical behavior of GMRES for solving singular systems of linear equations. It is well-known that the ill-conditioning of the extended Hessenberg matrix in the Arnoldi decomposition may affect the accuracy of computed approximate solutions in the GMRES method. We first recall the results obtained for range-symmetric and group projection matrices, and then extend them to matrices with general index. Theoretical results are accompanied with numerical experiments on small model problems.

Oblique projections in deflating GMRES type methods

Matthias Bolten (*Bergische Universität Wuppertal, Germany*)

16:50

Nemanja Bozovic (*Bergische Universität Wuppertal, Germany*)

Andreas Frommer (*Bergische Universität Wuppertal, Germany*)

When using restarts or solving several systems (possibly with varying matrices), acquiring information on certain eigenpairs and then deflating the corresponding components during the iterations can significantly accelerate the iteration process. Typically, orthogonal projections are used to perform these deflations. For sparse matrices, deflation can become quite costly since for each vector one has to compute one inner product and a SAXPY update.

In this talk we consider the use of oblique projections for deflation. These can be obtained by extracting approximations to left and right eigenvectors simultaneously. The advantage is that we then don't need to perform deflation in every step, but only every once in a while. We will present results from a number of numerical experiments.

Augmentation of Krylov subspaces for Lyapunov equations

Kirk Soodhalter (*Trinity College Dublin, Ireland*)

17:10

Krylov subspaces have been shown to be effective in a variety of applications involving large, sparse matrices, such as inexpensively computing the action of matrix functions and constructing low-rank solutions of large-scale matrix equations. Augmented Krylov subspace methods are a class of methods which have been quite successfully in accelerating the convergence of methods for solving linear systems by augmenting an iteratively generate Krylov subspace with some subspace containing "helpful" information. In this talk, we develop a subspace augmentation schemes compatible with obtaining a low-rank approximation to the solution of Lyapunov equations, with low-rank right-hand side.

We discuss additional hurdles which must be overcome in this setting so that these techniques can be applied for realistic problem dimensions. We discuss challenges such as proper augmentation of an extended Krylov subspace as well as how we properly project Lyapunov equations onto a sum of subspaces resulting from the augmentation process such that the resulting method can be implemented efficiently and is effective.

Shifted block FOM with restarts and low-rank modifications

Kathryn Lund (*École Polytechnique Fédérale de Lausanne, Switzerland*)

17:30

Andreas Frommer (*Bergische Universität Wuppertal*)

Daniel B. Szyld (*Temple University*)

An expansion of the generalized block Krylov subspace framework of [Electron. Trans. Numer. Anal., 47 (2017), pp. 100-126] is presented that allows for low-rank modifications of shifted block FOM (BFOM) with restarts. It is shown that block GMRES (BGMRES) and a new method, block Radau-Lanczos (BRL), are precisely such modifications of BFOM. A brief derivation of block Gauss and Gauss-Radau quadrature rules within the generalized framework are provided for BRL, showing that it can be used to prescribe Ritz values. Numerical results comparing BFOM, BGMRES, and BRL with different block inner products are presented for a variety of linear systems. The shifted modified BFOM framework is additionally used to develop new methods for approximating matrix functions acting on block vectors. Numerical results show that the BGMRES and BRL methods for matrix functions can significantly reduce the number of restart cycles needed for convergence. In particular, the BRL modification may eliminate the need for deflation in the case of linear dependence among the columns of the basis block vectors.

Approximation of the trace of matrix functions based on decay bounds

Claudia Schimmel (*Bergische Universität Wuppertal, Germany*)

17:50

Andreas Frommer (*Bergische Universität Wuppertal, Germany*)

The computation of the trace of functions of sparse matrices is an important task in numerous applications. Commonly, for sparse matrices A , the matrix $f(A)$ exhibits a rapid decay away from the sparsity pattern of A , such that many entries of $f(A)$ are very small in magnitude. Based on this observation, we present a method for approximating the trace of $f(A)$.

The method requires decay bounds for the entries of $f(A)$ and graph coloring algorithms and then computes just a few bilinear forms to determine an approximation of the trace of $f(A)$. The algorithm is compared to previously proposed and the effectiveness of this approach is shown in numerical experiments.

Automated local Fourier analysis (aLFA)

Karsten Kahl (*Bergische Universität Wuppertal, Germany*)

18:10

Nils Kintscher (*Bergische Universität Wuppertal, Germany*)

Local Fourier analysis (LFA) is a powerful tool used in the construction and analysis of multigrid methods. The fundamental idea of LFA is to leverage the connection between position space and frequency space via the Fourier transform. That is, in case the involved operators can be described by stencils in position space, i.e., they possess a shift invariant structure, their Fourier transform yields so-called symbols, which can be handled much more easily.

LFA yields exact convergence rates for multigrid methods applied to problems with periodic boundary conditions and yields good estimates in case other boundary conditions are employed and appropriate additional processing is applied. Due to this fact, LFA is one of the main tools in the quantitative analysis of two- and multi-grid methods.

In this talk we present an approach to LFA, which requires minimal user input by heavily exploiting the position space information. To do so we introduce a mathematical framework for the analysis of translationally invariant operators which alter value distributions on arbitrary repetitive structures, i.e., on lattices or crystals. As it turns out these structures are particularly well suited for building and analyzing multigrid methods. Our framework is developed to such an extent that the only task required of the user is to provide a description of the occurring operators with respect to (potentially non-matching) descriptions of the underlying repetitive structures.

In contrast to previously developed LFA we explicitly include the connection of the operator to the underlying structure. This allows us on one hand to easily manipulate operators in position space, e.g., by finding a least common lattice of two operators and rewriting their representation accordingly. On the other hand, this focus on structure yields a natural representation and discretization of the dual space that enables a full automation of the frequency space part of the analysis. We show that all these tasks can be carried out using basic principles and normal forms of integer linear algebra.

S17.06 | Applied and numerical linear algebra

Date: February 21, 2019

08:30-10:30

Room: Elise-Richter HS

Approximating with random rank-one vectors

Daniel Kressner (*EPFL, Switzerland*)

08:30

Randomized algorithms are becoming increasingly popular in numerical linear algebra and in scientific computing at large. One particularly convincing example is the approximation of the range and other quantities of a matrix A by multiplying A with a few Gaussian random vectors. The aim of this talk is to illustrate the usefulness of imposing further structure, specifically rank-one structure, on each of these random vectors. On the one hand, imposing such structure significantly complicates the analysis of algorithms, but on the other hand it can also reduce the complexity of randomized algorithms, sometimes drastically. The latter will be illustrated with several examples, ranging from condition number estimation for matrix functions to low-rank tensor compression.

Approximate interpolation of high dimensional, scattered data in tree tensor formats

Sebastian Kraemer (*RWTH Aachen, Germany*)

08:50

Lars Grasedyck (*RWTH Aachen, Germany*)

Multivariate approximate interpolation of scattered data is a highly ill-posed inverse problem and requires a suitable model with adaptive complexity in order to solve it. We explore the benefits of combining classical smoothness properties with more recent algebraic low-rank features, known for their resistance to the curse of dimensionality.

In particular, we extend the well known thin-plate spline least squares regression to high dimensions through the use of tree tensor formats. For example, the algebraic tensor products preserves the continuity of monovariate, second order Sobolev spaces. On the other hand, the bilinear form realizing the thin-plates penalty term has rank three, regardless of the chosen format.

The resulting challenge of rank adaption is an essential part, yet heuristics are often bound to fail due to a certain type of instability in multilinear optimization. Using a singular value based stabilization term, this issue can however be successfully be handled.

Furthermore, the use of coarse CG allows to obtain optimal computational complexity in each microstep. We apply the algorithm to the regression of pass schedule data, in which the tree format can be chosen according to the physical interpretation behind the input parameters.

Hybrid compression of high-frequency Helmholtz integral operators

Steffen Börm (*CAU Kiel, Germany*)

09:10

Christina Börst (*CAU Kiel, Germany*)

Boundary element methods typically lead to large densely populated matrices. Compression techniques like the fast multipole method or ACA can be applied to significantly reduce the storage requirements, allowing us to handle high-resolution meshes efficiently.

In the case of the Helmholtz boundary integral equation at high frequencies, the kernel function oscillates rapidly, and this leads to slow convergence of standard compression techniques.

We propose a hybrid approach that combines directional interpolation with algebraic recompression. Directional interpolation splits the kernel function into a plane wave and a smooth remainder, and since the remainder can be approximated efficiently, combining the interpolating polynomial with the plane wave gives rise to a fast approximation scheme.

Although fast, directional interpolation considered on its own is not particularly useful, since it requires a very large amount of storage. We address this issue by applying a recompression algorithm that exploits low-rank properties of the matrix in order to significantly reduce the storage requirements, while the runtime is only moderately increased.

Numerical experiments illustrate that the new algorithm has almost linear complexity and that the recompression preserves the fast convergence of the underlying interpolation scheme.

An algorithm for computing the restricted singular value decomposition with improved robustness

Ian Zwaan (*Bergische Universität Wuppertal, Germany*)

09:30

The singular value decomposition (SVD) of a matrix A is a well-known and widely used matrix decomposition. There are several useful generalizations of the SVD with the most notable example being the quotient SVD (QSVD) of a matrix pair (A, C) . In fact, usage of the QSVD is widespread enough that it is often called “the” generalized SVD (GSVD), despite the inherent

ambiguity. A lesser known generalization is the restricted SVD (RSVD) of a matrix triplet (A, B, C) . Unfortunately, current numerical methods for computing the RSVD (Zha; Chu, De Lathauwer, and De Moor) require a number of inter-dependent rank decisions in their preprocessing steps. Due to round-off errors and the fact that rank decisions are ill-posed, these steps are prone to failure, especially if QR with pivoting is used instead of the SVD for the rank decisions. We present a new method that only requires three rank decisions in the preprocessing steps, and where the second and third are independent of each other. Like Zha's algorithm, our algorithm performs a Kogbetliantz-type iterations after the preprocessing phase. An essential part of these iterations is a 2×2 RSVD of three upper-triangular matrices. In order to improve robustness, we additionally discuss a new 2×2 RSVD algorithm that is backward stable.

A low-rank tensor method for optimal control of fractional PDEs

Gennadij Heidel (*Trier University, Germany*)

09:50

Venera Khoromskaia (*MPI for Mathematics in the Sciences, Germany*)

Boris Khoromskij (*MPI for Mathematics in the Sciences, Germany*)

Volker Schulz (*Trier University, Germany*)

Modelling, simulation and optimization of systems governed by fractional and nonlocal PDEs have attracted considerable interest in recent literature. The non-locality of the operator leads to a dense discretized system. This presents a major difficulty for standard solvers, since the solution of large, dense problems is computationally very expensive. We present a method to overcome these for a fractional Laplacian control problem by exploiting well-known approximation results for the underlying operator and extending them to the control case. In the discrete case on tensor grids, these properties lead to a low Kronecker rank structure, which allows a cheap computation of matrix-vector products. We use this structure to construct a direct solver for the optimal control problem, whose computational complexity is independent of the problem dimension. We show our novel approach to outperform existing standard methods.

Block partitioning of sparse rectangular matrices

Andrei-Alin Dumitrasc

(*Friedrich-Alexander-Universität Erlangen-*

10:10

Nürnberg, Germany)

Philippe Leleux (*Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique, Toulouse, France*)

Ulrich Rüde (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

The Augmented Block Cimmino Distributed (ABCD) method is a hybrid solver used for large, sparse, consistent systems of linear equations, which are solved by extending the matrix such that the resulting block-row partitions lead to orthogonal subspaces. In order to minimize the size of this extension, it is important to reorder the matrix using an algorithm such as Reverse Cuthill-McKee (RCM), which attempts to bring the nonzeros closer to the diagonal, generating a block tridiagonal structure. In the original paper, ABCD is analyzed mostly from the perspective of square matrices, for which RCM can be readily used. Our work focuses on the case of rectangular matrices, and how RCM can be altered such that it can be applied here, using a connection with bipartite graphs. The reordered matrix has a block bidiagonal structure and can then be fed to ABCD. Such developments can also be useful in the broader context of inconsistent systems of linear equations.

S17.07 | Applied and numerical linear algebra

Date: February 22, 2019

08:30-10:30

Room: Elise-Richter HS

A subspace framework for H-infinity-norm minimization

Nicat Aliyev (*Istanbul Sabahattin Zaim University, Turkey*)

08:30

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*)

Emre Mengi (*Koc University, Turkey*)

Matthias Voigt (*Technische Universität Berlin, Germany*)

In this talk we discuss the minimization of the H-infinity-norm of a large-scale parametrized descriptor system over a set of admissible parameter values. We propose a greedy and interpolatory subspace framework for this minimization problem which is inspired by our recent work [Aliyev et al., SIAM J. Matrix Anal. Appl., 38(4):1496-1516, 2017] for the computation of the H-infinity-norm. Our algorithm minimizes the H-infinity-norm of a reduced-order parametrized system obtained by two-sided Petrov-Galerkin projections onto certain subspaces. Then it expands the subspaces so that Hermite interpolation properties hold between the full and reduced-order parametrized system at the optimal parameter value for the reduced-order system. We discuss the superlinear rate of convergence of this method and illustrate its behavior by several examples.

Projected Newton-Kleinman method for the algebraic Riccati equation

Davide Palitta (*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*)

08:50

The numerical solution of the algebraic Riccati matrix equation $AX + XA^T - XBB^T X + C^T C = 0$, where $A \in R^{n \times n}$, $B \in R^{n \times m}$, $C \in R^{p \times n}$, $p + m \ll n$, is an interesting and still challenging task especially when the problem dimension is very large, say $n > 10^4$, as the dense solution X cannot be store and a memory-saving approximation has to be sought.

In general, the Riccati equation has many solutions but, under certain conditions on the coefficient matrices A , B and C , there exists a unique stabilizing solution, that is all the eigenvalues of the matrix $A - BB^T X$ have negative real part.

One of the most classical iterative methods for the computation of such an X is the so-called Newton-Kleinman method that, given a stabilizing initial guess X_0 , computes an approximation X_{k+1} to X by sequentially solving Lyapunov equations of the form

$$(A - X_k BB^T)X_{k+1} + X_{k+1}(A - X_k BB^T)^T + C^T C + X_k BB^T X_k = 0.$$

Due to the problem dimension, these equations must be iteratively solved, leading to the inexact Newton-Kleinman method which provides a low-rank approximation to X .

Other very efficient methods have been developed in the last years. In particular, it has been shown that projection methods are very effective in the numerical treatment of Riccati equations and they straightforwardly generalize the approach used for linear matrix equations. However, to the best of our knowledge, it is not guaranteed that the solution computed by projection methods is the stabilizing solution.

In this talk we present a novel approach that combines the inexact Newton-Kleinman scheme with projection methods for Lyapunov equations. In particular, we show that all the iterates X_{k+1} in

Newton scheme belong to the same space used to compute X_1 , so that only one approximation space has to be constructed. This leads to remarkable reductions in the computational efforts. Moreover, the well-established convergence properties of the inexact Newton-Kleinman method are preserved.

Several numerical results are reported to illustrate the potential of the discussed method.

Efficient preconditioning of hp-FEM matrices by hierarchical low-rank approximations

Paolo Gatto (*RWTH University, Germany*)

09:10

Jan S Hesthaven (*Ecole Polytechnique Federale de Lausanne, Switzerland*)

In this talk I will introduce a preconditioner based on low-rank compression of Schur complements. The construction is inspired by the well-known nested dissection strategy, and relies on the assumption that the Schur complements that arise in the elimination process can be approximated, to high precision, by compressible matrices. The preconditioner is built as an approximate LDM^T factorization of a given matrix A , and no knowledge of A in assembled form is required by the construction. The LDM^T factorization is amenable to fast inversion, and the inverse can be applied fast as well. I will present numerical experiments that investigate the behavior of the preconditioner in the context of Discontinuous Galerkin finite element approximations of positive-definite problems, as well as indefinite wave propagation problems.

Low rank tensor train methods for isogeometric analysis in PDE-constrained optimization

Alexandra Buenger (*Technical University Chemnitz, Germany*)

09:30

Martin Stoll (*Technical University Chemnitz, Germany*)

Sergey Dolgov (*University of Bath, United Kingdom*)

Isogeometric analysis (IgA) is a popular method for the discretization of partial differential equations motivated by the use of NURBS (Non-uniform rational B-splines) for geometric representations in industry and science.

In IgA the domain representation as well as the discrete solution of a PDE are described by the same global spline functions. However, the use of an exact geometric representation comes at a cost. Due to the global nature and large overlapping support of the basis functions, system matrix assembly becomes especially costly in isogeometric analysis.

To reduce the computing time and storage requirements low-rank tensor methods have become a promising tool. We successfully constructed a framework applying low rank tensor train calculations to IgA to efficiently solve PDE-constrained optimization problems on complex three dimensional domains without assembly of the actual system matrices. The method exploits the Kronecker product structure of the underlying spline space, reducing the three dimensional system matrices to a low-rank format as the sum of a small number of Kronecker products $M = \sum_{i=1}^n M_i^{(1)} \otimes M_i^{(2)} \otimes M_i^{(3)}$, where n is determined by the chosen size of the low rank approximation. For assembly of the smaller matrices $M_i^{(d)}$ only univariate integration in the corresponding geometric direction d is performed, thus significantly reducing computation time and storage requirements.

The developed method automatically detects the ranks for a given domain and conducts all necessary calculations in a memory efficient low rank tensor train format. We present the applicability of this framework to efficiently solve various large scale PDE-constrained optimization problems using the iterative *AMEn block solve* algorithm which preserves and exploits the low rank format of the system matrices.

Scalable parallel hierarchical matrices on GPUs

Peter Zaspel (*University of Basel, Switzerland*)

09:50

In this work, we study the scalable parallelization of hierarchical (H) matrix algorithms on clusters of graphics processing units. H matrices approximate specific dense matrices, e.g., from discretized integral equations or kernel ridge regression, leading to log-linear time complexity in dense matrix-vector products. While the parallelization of H matrix operations on a single GPU has been considered by the author before (and resulted in the Open Source library "hmglib"), the next important step is to parallelize these algorithms over many GPUs. Here, the crucial challenges are (1) an efficient load balancing between the GPUs, (2) an efficient use of the very limited GPU memory resources and (3) a good to excellent scalability of the algorithms in presence of the relatively slow interconnect between the GPUs.

The presentation will show the latest results of this multi-GPU parallelization effort in context of an application in boundary integral equations.

This work is partially based on joint work with Helmut Harbrecht.

The Loewner framework for modeling and analysis of nonlinearities in the context of Generalized Frequency Response Functions

Dimitrios Karachalios (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

10:10

Ion Victor Gosea (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Athanasios C. Antoulas (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany, Rice University, USA, Baylor College of Medicine, USA*)

One of the main approaches to model reduction of both linear and non-linear dynamical systems is by means of interpolation. Such approaches seek reduced models whose transfer function matches that of the original system at selected interpolation points. A particular class is represented by data-driven methods which are the topic of interest in this work. The primary method, which will be referred to as the Loewner framework, was originally introduced by the third author. It constructs models from given data sets (pairs of sample points and samples values) naturally and in a straightforward manner. Its primary attribute is that it provides a trade-off between the accuracy of fit and complexity of the reduced model. Through this framework, one can derive state-space models directly from input-output data without requiring any realization of the system. In the linear case, the Loewner framework is purely data-driven and constructs a reduced order model (ROM) from measurements of the transfer function. Results regarding approximations of non-rational functions and construction of ROMs by compression, adaptive/optimal selection are presented. In the class of bilinear systems and quadratic-bilinear systems, the Loewner framework has been already extended in the concept of the Generalized Frequency Response Functions (GFRFs). In this direction, the current work includes a study that correlates the GFRFs which are derived from the above extensions of the Loewner framework with the classical approach by Volterra series. The scope of the proposed methodology is to address procedures that experimentally exploit high fidelity models. These could be used for solving industrial engineering problems.

S18 | Numerical methods of differential equations

Organiser: Ilaria Perugia (*University of Vienna, Austria*)
Mario Ohlberger (*University of Münster, Germany*)

S18.01 | Numerical methods of differential equations

Date: February 19, 2019
Room: HS 31

08:30-10:30

Localization and mass conservation in reduced basis methods

Felix Schindler (*WWU Münster, Germany*)
Mario Ohlberger (*WWU Münster, Germany*)

08:30

In the context of parameterized partial differential equations (PPDE), we consider projection-based model order reduction by Reduced Basis methods (RB), see [Benner, P., Ohlberger, M., Patera, A., Rozza, G., and Urban, K. (eds.) (2017). *Model Reduction of Parametrized Systems*. Springer-Verlag GmbH. doi:10.1007/978-3-319-58786-8.] and the references therein. The resulting reduced order models (ROM) allow for an efficient and accurate approximation of the PPDEs solution (or a derived quantity) in real-time or many query contexts (such as inverse problems or optimal control).

For some PDEs, however, it is in addition desirable that basic properties of the solution (such as energy stability or local mass conservation) carry over to the approximate solution; while usually ensured by the underlying discretization this is by no means guaranteed by ROMs and subject of ongoing research (see for instance [Mohebujjaman, M., Rebholz, L.G., Xie, X., and Iliescu, T. (2017). *Energy balance and mass conservation in reduced order models of fluid flows*. *J. Comput. Phys.*, 346, 262-277.] and [Abdulle, A. and Budac, O. (2017). *A discontinuous Galerkin reduced basis numerical homogenization method for fluid flow in porous media*. *SIAM J. Sci. Comput.*, 39(1), A83-A113. doi:10.1137/15M1050690.]).

To the best of our knowledge, the localized RB multi-scale method (LRBMS), introduced in [Albrecht, F., Haasdonk, B., Kaulmann, S., and Ohlberger, M. (2012). *The localized reduced basis multiscale method*. In *Proceedings of Algorithm 2012, Conference on Scientific Computing, Vysoke Tatry, Podbanske, September 9-14, 2012*, 393-403. Slovak University of Technology in Bratislava, Publishing House of STU.] and [Ohlberger, M. and Schindler, F. (2015). *Error Control for the Localized Reduced Basis Multiscale Method with Adaptive On-Line Enrichment*. *SIAM J. Sci. Comput.*, 37(6), A2865-A2895. doi:10.1137/151003660.] as a combination of RB and domain decomposition (DD) methods, can be considered the first method to ensure local mass conservation of ROMs w.r.t. the DD in the context of RB methods. We present recent advances in the context of the LRBMS and of mass conservation in the context of RB methods for elliptic problems, in particular regarding a posteriori error control and locally mass conservative flux reconstructions, based on [Ern, A., Stephansen, A.F., and Vohralik, M. (2010). *Guaranteed and robust discontinuous galerkin a posteriori error estimates for convection-diffusion-reaction problems*. *J. Comput. Appl. Math.*, 234(1), 114-130.].

A technique for rational model order reduction of parametric problems lacking uniform inf-sup stability

Davide Pradovera (*EPFL, Switzerland*)
Francesca Bonizzoni (*University of Vienna, Austria*)
Fabio Nobile (*EPFL, Switzerland*)
Ilaria Perugia (*University of Vienna, Austria*)

08:50

In this talk we consider parametric PDEs whose operators lack uniform inf-sup stability over the parametric domain. In particular, we assume that the solution map of the problem (which associates each parameter with the corresponding solution of the PDE, if it exists) is meromorphic. Among the consequences of this assumption, we observe that the locus of “resonances” of the problem, i.e. the set including all those parameters for which the PDE is unstable, must display a certain regularity.

Exploiting this property, we develop a model order reduction technique for the approximation of this class of problems:

- in the offline phase, snapshots of the solution of the PDE or of its derivatives with respect to the parameter are computed in a (Lagrange, Taylor, or Hermite) Reduced Basis-type framework;
- the reduction step, instead of consisting in a Galerkin projection of the problem over a suitable subspace, aims at approximating the resonant set through the solution of a convex optimization problem based on the snapshots;
- the approximation of the solution map is then obtained through a Least-Squares interpolation of the data, with the final result being a rational function whose dependence on the parameter is explicit, and whose evaluation online can be performed very efficiently.

The crucial step of the algorithm is the solution of the optimization problem which allows to approximate the resonances of the PDE. In the literature of rational approximation, a linearized version of the residual is often chosen as target of the optimization. In our technique, we follow a modified approach, obtained through a further simplification of the residual, allowing for a less costly algorithm. Adopting such functional, we present several theoretical results concerning the convergence of the approximate solution map and of the resonant set, under some spectral assumptions on the operator of the parametric problem.

As numerical examples to verify our claims, we consider an external scattering problem with parametric wavenumber, as well as an internal scattering problem with parameter-dependent domain.

Model order reduction for space-adaptive simulations of unsteady incompressible flows

Carmen Gräßle (*Universität Hamburg, Germany*)

09:10

Michael Hinze (*Universität Hamburg, Germany*)

Jens Lang (*Technische Universität Darmstadt, Germany*)

Sebastian Ullmann (*Technische Universität Darmstadt, Germany*)

We consider model order reduction for unsteady incompressible Navier-Stokes problems. A reduction of computational complexity is achieved by a Galerkin projection of the solution of a high-dimensional reference problem onto a low-dimensional subspace. We focus on subspaces generated by a proper orthogonal decomposition (POD) of space-adapted finite element snapshots. In previous works, we have investigated adaptive POD-Galerkin modeling for elliptic and parabolic problems [1,2]. Incompressible flows pose additional challenges regarding the stability of the resulting reduced-order models and regarding the implementation of inhomogeneous initial and boundary condition.

We propose two approaches to computing reduced spaces which result in stable POD-Galerkin models. The first approach employs a projection of the adapted velocity snapshots onto a space of functions which are weakly divergence-free with respect to a pressure reference space. The resulting reduced-order model is a system of ordinary differential equations for the velocity POD coefficients. The second approach is based on separate PODs of the adapted velocity and pressure snapshots. Here, the velocity POD basis is enriched by supremizer functions computed on a reference velocity space. The stability of the velocity-pressure pair of reduced spaces is linked to the inf-sup constant of the reference discretization.

We analyze the complexity of the proposed reduced-order models, present numerical results for a benchmark problem, and compare our methods in terms of accuracy per computational cost.

References

- [1] C. Gräßle and M. Hinze, POD reduced-order modeling for evolution equations utilizing arbitrary finite element discretizations, *Adv. Comput. Math.* (2018), doi: 10.1007/s10444-018-9620-x.
- [2] S. Ullmann, M. Rotkvic and J. Lang, POD-Galerkin reduced-order modeling with adaptive finite element snapshots, *J. Comput. Phys.* (2016), 325:244-258, doi: 10.1016/j.jcp.2016.08.018.

Towards efficient band structure computations of photonic crystals using model order reduction

Marine Froidevaux (*TU Berlin, Germany*)

09:30

Photonic crystals are composite materials having a periodic structure which affects the propagation of light. We are interested in analyzing the optical characteristics of multiple photonic crystal types by computing their so-called band diagram, i.e. the graph of the eigenfrequencies versus the wavevector.

In order to build these band diagrams for some given parameter values, multiple large-scale nonlinear eigenvalue problems derived from the Maxwell equations need to be solved. In this talk, we will present some numerical results obtained by applying a POD-based model order reduction method to the parametric eigenvalue problem.

Multi-fidelity optimization using reduced order models

Kevin Allen Tolle (*Trier University, Germany*)

09:50

Nicole Marheineke (*Trier University, Germany*)

Optimal control problems constrained to nonlinear partial differential equations (PDEs) appear in many applications. These problems prove to be computationally expensive to solve because the discretizations of the PDEs result in large-scale problems. Therefore, a direct solution approach is not always viable. We consider the aggressive space-mapping approach using surrogate models derived with the help of model order reduction techniques in order to efficiently solve such problems, while maintaining an acceptable accuracy. Numerical results based on a medical application (laser-induced thermotherapy) are used to evaluate the effectiveness of the proposed approach.

Generalized Galerkin approximation in time for wave equations

Markus Bause (*Helmut Schmidt University Hamburg, Germany*)

10:10

Mathias Anselmann (*Helmut Schmidt University Hamburg, Germany*)

Information on wave propagation on all scales continues to remain of importance in several branches of natural sciences and technology. Therefore, progress in the numerical modeling of wave phenomena is desirable. Here, we present generalized families of variational space-time finite element methods for the numerical approximation of solutions to wave problems; cf. [1,3]. The schemes combine the concepts of collocation methods and variational formulations for the discretization of the time variable. In particular, the schemes enhance the global regularity in time of the fully discrete approximation to higher-order differentiability. For instance, this can be exploited in the discretization of coupled problems of multiphysics. Moreover, a computationally cheap post-processing operator (cf. [2,4]) that further lifts the regularity in time of the fully discrete approximation and increases the order of convergence is introduced. The post-processing can be used for a-posteriori error control and space-time mesh adaptivity. For the discretization of the space variables discontinuous Galerkin methods are applied.

Results of the analysis of the schemes including optimal-order error estimates are presented; cf. [2]. Moreover, their performance properties are illustrated by various numerical experiments of different complexities; cf. [1,4]. Finally, the technology of the linear solver for the arising complex block systems is discussed.

References

- [1] M. Anselmann, M. Bause, Numerical study of Galerkin approximation with higher-order regularity in time for wave equations, in preparation, 2018.
- [2] M. Bause, U. Köcher, F. A. Radu, F. Schieweck, Post-processed Galerkin approximation of improved order for wave equations, *Math. Comp.*, submitted (2018), arXiv:1803.03005, pp. 1-34.
- [3] S. Becher, G. Matthies, D. Wenzel, Variational methods for stable time discretization of first-order differential equations, Preprint TU Dresden (2017), pp. 1-13.
- [4] U. Köcher, M. Bause, Variational space-time methods for the wave equation, *J. Sci. Comput.*, 61 (2014), pp. 424-453.

S18.02 | Numerical methods of differential equations

Date: February 19, 2019

16:30-18:30

Room: HS 06

Tensor methods for the time-dependent Vlasov-Poisson system

Virginie Ehrlicher (*Ecole des Ponts Paristech & INRIA, France*)

16:30

Damiano Lombardi (*Ecole des Ponts Paristech & INRIA, France*)

A numerical method will be presented to solve the full-Eulerian time-dependent Vlasov-Poisson system in high dimension. The algorithm relies on the construction of a tensor decomposition of the solution whose rank is adapted at each time step. This decomposition is obtained through the use of an efficient modified Progressive Generalized Decomposition (PGD) method, whose convergence is proved. We suggest in addition a symplectic time-discretization splitting scheme that preserves the Hamiltonian properties of the system. This scheme is naturally obtained by considering the tensor structure of the approximation. The efficiency of this approach will be illustrated through time-dependent 3D-3D numerical examples.

A domain decomposition method for the Poisson-Boltzmann solvation model

Chaoyu Quan (*Sorbonne Université, France*)

17:10

Benjamin Stamm (*RWTH Aachen University, Germany*)

Yvon Maday (*Sorbonne Université, France*)

In this talk, we present a domain decomposition method for the Poisson-Boltzmann (PB) solvation model that is widely used in computational chemistry. This method solves the linear Poisson-Boltzmann (LPB) equation defined on the entire unbounded three-dimensional domain using the van der Waals cavity as the solute cavity. The Schwarz domain decomposition method, in combination with an integral equation formulation, is used to formulate local problems by decomposing the cavity into overlapping balls and only solving a set of coupled sub-equations in balls. A series of numerical experiments are presented to test the robustness and the efficiency of this method including the comparisons with some existing methods. We observe exponential convergence of the solvation energy with respect to the number of degrees of freedom which allows this method to reach an accuracy required when coupling with quantum mechanical descriptions of the solute.

Efficient numerical methods for nonlinear DAEs arising from gas transportation networks

Nicodemus Banagaaya (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*) 17:30
Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Gas transportation networks can be modeled by the isothermal Euler equations and, spatial discretization of these equations leads to large-scale systems of nonlinear differential algebraic equations (DAEs). We are interested in a fast and stable prediction of the dynamics of natural gas transport in the pipe networks, and therefore an efficient numerical method is vital. DAEs are known to be difficult to simulate and the level of difficulty is measured using index concepts such as differential index, tractability index, etc. The higher the index, the more difficult to simulate the DAE. Moreover, the underlying PDE is hyperbolic leading to increased computational complexity. Depending on the topology of the network, systems are of tractability index at most 2, and they are of tractability index 2 if and only if they have more than one supply input. Existing techniques rewrite such systems as ordinary differential equations (ODEs), then standard numerical methods such as implicit-explicit numerical methods, are employed. However, this affects the choice of the numerical solver strongly, and sometimes these models are computationally expensive especially if the index is higher than 1. We propose a numerical method for nonlinear DAEs arising from gas transportation networks which involve automatic decoupling of nonlinear DAEs into nonlinear ODEs and algebraic equations, then the standard numerical techniques can be applied separately on both the differential and algebraic parts. This leads to fast simulation of gas transportation networks. We illustrate the performance of our numerical method on benchmark problems of gas networks and the numerical results show the advantage of our method.

Parallel tensor arithmetic in the Hierarchical Tucker format

Christian Löbber (*RWTH Aachen, Germany*) 17:50
Lars Grasedyck (*RWTH Aachen, Germany*)

We use the Hierarchical Tucker format (HT-format) to represent high-dimensional tensors with a complexity that grows linearly with the tensor order d , provided that certain low-rank structures are present in the tensor data. The library developed by us in C++/MPI makes it possible to store the tensor data distributed on several compute nodes. For such distributed stored tensors in the HT-format we have developed parallel algorithms that perform arithmetic operations like dot products, orthogonalization, truncation or matrix-vector products. Due to the tree structure of the HT-format, the parallel runtime of our algorithms grows like $\log(d)$ instead of the sequential $O(d)$ dependency.

We apply these algorithms in iterative methods, such as calculating or even finding maximal entries in tensors.

A SDE waveform-relaxation method with application in distributed neural network simulations

Jan Hahne (*University of Wuppertal, Germany*) 18:10
Matthias Bolten (*University of Wuppertal, Germany*)

Waveform-relaxation methods are a set of iterative methods to solve systems of differential equations by dividing them into subsystems. Several of these methods, such as the Jacobi waveform-relaxation method, enable potential for parallelization across the system and are for that reason interesting in applications with a highly parallel setting. Here we present a SDE waveform-relaxation methods with applications in the fields of computational neuroscience. We analyze how and where the application of the method can speed up the simulation of functionally inspired rate-based units in a distributed neural network simulator that was originally designed for biologically grounded spiking neuron models. Such a unified simulation framework supports the combination of the two approaches for multi-scale modeling and enables the quantitative validation of mean-field approaches by spiking network simulations.

S18.03 | Numerical methods of differential equations

Date: February 20, 2019

08:30-09:30

Room: HS 31

A study of scaled boundary parametrizations in isogeometric analysis

Clarissa Arioli (*TU Kaiserslautern, Germany*)

08:30

Bernd Simeon (*TU Kaiserslautern, Germany*)

This contribution is concerned with scaled boundary parametrizations for Isogeometric Analysis (IGA). These are easy to construct and advantageous if only a boundary description of the computational domain is available. The idea goes back to the Scaled Boundary Finite Element Method [3], which has then been extended to IGA. We here study these parametrizations as bivariate or trivariate B-spline functions that are directly suitable for standard Galerkin-based IGA.

In the talk, the relation of this approach to the classical concept of Isogeometric Analysis is analyzed. In particular, focusing on a linear problem, we compare classical IGA with scaled boundary IGA where the weak form and Galerkin projection are used both in scaling and in circumferential direction. Using the Poisson equation as example, we explain the relation between these two methods by means of the Laplace-Beltrami operator. Additionally the singularity in the scaling center is here investigated with regard to numerical integration.

This work is supported by the DFG within the project "Hybrid Galerkin-collocation methods for surface-oriented modeling of nonlinear problems in solid mechanics".

References:

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- [2] L. Chen, B. Simeon and S. Klinkel, A NURBS based Galerkin approach for the analysis of solids in boundary representation. *Computer Methods in Applied Mechanics and Engineering* 305, 777–805, 2016.
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Optimal enforcement of Dirichlet conditions on curvilinear boundaries for Lagrange and Hermite finite element methods with straight-edged simplexes

Vitoriano Ruas (*Sorbonne Université, France*)

08:50

The finite element method is a versatile technique to deal with different types of geometries. This is particularly true of problems posed in curved domains of arbitrary shape. In the case of second-order boundary-value problems with Dirichlet conditions prescribed on curvilinear boundaries,

method's isoparametric version for meshes consisting of curved triangles or tetrahedra has been mostly employed. Its aim is to recover the optimal approximation properties known to hold for methods of order greater than one based on standard straight-edged elements, in the case of polygonal or polyhedral domains. However, besides algebraic and geometric inconveniences, the isoparametric technique is limited in scope, since its extension to degrees of freedom other than function values is not straightforward.

In this work we present a simple alternative bypassing the above drawbacks, without eroding qualitative approximation properties. The proposed technique can do without curved elements and is based only on polynomial algebra. It is first illustrated in the case of the convection-diffusion equation solved with standard Lagrange elements. Then it is applied to the solution of fourth-order equations with Dirichlet conditions by means of Hermite elements having normal-derivatives as degrees of freedom.

Unstructured T-splines based on local higher-dimensional mesh representations

Philipp Morgenstern (*Leibniz Universität Hannover, Germany*)

09:10

Roland Maier (*Universität Augsburg, Germany*)

In 2003, T-splines were introduced in the context of CAD as a new realization for B-splines on irregular meshes that does not require the bookkeeping of a hierarchical basis, but nevertheless allows for local mesh refinement in order to control small-scale geometry features. Shortly after, IGA was introduced, and T-splines were applied with promising results, but were at the same time proven to lack linear independence in certain cases, which actually excludes them from the application in a Galerkin method. Another algorithmic difficulty was revealed in 2011, namely that a naive refinement strategy may not only yield linear dependencies between the shape functions, but also non-nested spline spaces, which compromises the theoretical approximation properties of the method as well as the preservation of exact geometry data during refinement. The issue on linear independence was solved in 2012 with the insight that linear independence is guaranteed if the T-junction extensions do not intersect (analysis-suitability). The second issue, namely how to generate nested spline spaces, was solved in a new refinement algorithm, also preserving linear independence of the T-splines. Still in 2012, new insight on the linear independence of T-splines was provided by introducing the more abstract concept of dual-compatibility and proving its equivalence to analysis-suitability, and in 2013, these concepts were generalized to T-splines of arbitrary polynomial degree, but still restricted to the two-dimensional case. Also at that time, techniques were introduced for the construction of 3D T-spline meshes from boundary representations, motivating the theoretical research on T-splines in three space dimensions, but in particular the linear independence of higher-dimensional T-splines was only characterized through the dual-compatibility criterion, until in 2016, the presenting author of this talk introduced a definition of T-junction extensions and analysis-suitability in three dimensions.

This talk proposes a construction of analysis-suitable T-splines for unstructured meshes with extraordinary nodes of valence 3. The construction locally uses higher-dimensional meshes of which the given unstructured mesh is a lower-dimensional projection. We address the local linear independence as well as the local mesh refinement for this kind of T-splines, accounting for the preservation of linear independence and quasi-nestedness of the spline spaces (quasi-orthogonality in the context of mesh-adaptive Galerkin schemes), and sketch ideas towards a theoretical rate-optimality for the application to a second-order elliptic PDE.

S18.04 | Numerical methods of differential equations

Date: February 20, 2019

14:00-16:00

Room: HS 31

Equivalence of local- and global-best approximations and simple stable local commuting projectors in $H(\text{div})$

Alexandre Ern (*Universite Paris-Est, France*)

14:00

Thirupathi Gudi (*Indian Institute of Science Bangalore, India*)

Iain Smears (*University College London, United Kingdom*)

Martin Vohralik (*Inria Paris, France*)

We prove, under minimal regularity, results permitting to localize the global-best approximations by $H(\text{div})$ -conforming finite element spaces. More precisely, we show that the global-best approximation of a given $H(\text{div})$ function in a $H(\text{div})$ -conforming finite element space imposing the normal trace continuity constraint can be bounded above and below by the sum of the respective local approximations from the elementwise local spaces without any inter-element continuity imposed along the interfaces. Applications of these results leading to optimal a priori error estimates that avoid any notion of an interpolation operator and apply under minimal regularity to mixed finite element and least-squares methods are presented. Incidentally, we construct a projector from $H(\text{div})$ to its conforming finite element subspace that is simultaneously locally defined (over patches of elements), simple as obtained via local-best approximation followed by “flux reconstruction”, commuting with the L^2 -projection, and stable in the L^2 norm.

Fast diagonalized Schwarz smoothers for geometric multigrid preconditioning on unstructured meshes

Julius Witte (*Heidelberg University, Germany*)

14:40

Daniel Arndt (*Heidelberg University, Germany*)

Guido Kanschat (*Heidelberg University, Germany*)

Efficiently solving linear equations resulting from finite element discretizations still poses a challenge and is subject of ongoing research. This talk aims to combine two techniques:

1. The matrix-free framework is tailored to state-of-the-art computer architectures, outperforming the common sparse matrix arithmetic, particularly for higher order finite elements.
2. A powerful preconditioner for linear problems is offered by a geometric multigrid algorithm having a favorable linear complexity if a suitable smoother is used. It is well-known that (overlapping) Schwarz smoothers using local spaces supported on patches of finite elements provide robust convergence for a wide range of problems.

The standard approach of assembling Schwarz smoothers is to extract the local stiffness matrices from the global system matrix which is not feasible in a matrix-free framework. Furthermore, Schwarz smoothers are expensive to compute and store, especially for higher order discontinuous Galerkin discretizations or local spaces supported on vertex patches. However, this is contradictory to the memory efficiency of the matrix-free idea. Exploiting the tensor product finite elements on the subproblem level offers a remedy to both. The local bilinear forms of the smoother do not have to match the global operator, such that we can approximate them by separable problems. First, we show how to reduce the complexity of inverting and storing subspace problems by means of the fast diagonalization method. Second, we illustrate the key idea of using sum-factorization for matrix-vector products resulting from the global forward problem as well as the local inverse problems. Finally, the efficiency of our proposed fast diagonalized Schwarz

smoothers is underlined by numerical experiments on Cartesian and non-Cartesian meshes. In particular, we demonstrate that the throughput, namely how many degrees of freedom can be processed per second, of the proposed smoothers is indeed comparable to the throughput of a matrix-free matrix-vector product.

Guaranteed a posteriori error analysis for the mixed Laplace eigenvalue problem

Fleurianne Bertrand (*Humboldt Universität zu Berlin, Germany*) 15:00
Daniele Boffi (*University of Pavia, Italy*)
Rolf Stenberg (*Aalto University, Finland*)

We present a reconstruction in the standard H^1 -conforming space for the primal variable of the mixed Laplace eigenvalue problem. This reconstruction is performed locally on a set of vertex patches. The resulting error estimator constitutes a guaranteed upper bound for the error and is shown to be local efficient.

Analysis of a boundary element method for homogenization of periodic structures

Günther Of (*Graz University of Technology, Austria*) 15:20
Dalibor Lukas (*VSB - Technical University of Ostrava, Czech Republic*)
Jiri Bouchala (*VSB - Technical University of Ostrava, Czech Republic*)
Jan Zapletal (*VSB - Technical University of Ostrava, Czech Republic*)

In case of multiply-connected domains, some properties of the boundary integral operators differ from the setting of simply-connected domains. In particular, the kernel and the ellipticity property of the hypersingular operator are different. We will discuss some details of the modifications in the analysis of boundary integral operators and of considered boundary integral formulations. A specific application is a homogenization method for periodic structures based on boundary element calculations in the periodic cell. A super-linear convergence of the homogenized coefficients can be proven by means of the above mentioned analysis and is observed in numerical examples.

On the numerical analysis of an integral equation formulation of the many-body dielectric problem in electrostatics

Muhammad Hassan (*RWTH Aachen University, Germany*) 15:40
Benjamin Stamm (*RWTH Aachen University, Germany*)

We consider the problem of calculating the electrostatic interaction between dielectric spheres embedded in a polarisable continuum. In order to solve this problem, E. Lindgren et al. (The Journal of Computational Physics, 2018) have proposed a numerical method based on a Galerkin discretisation of an integral equation formulation of this problem. The proposed method is general enough to treat any homogeneous dielectric medium containing an arbitrary number of spherical particles of any size, charge, dielectric constant and position in the three-dimensional space. Furthermore, numerical experiments indicate that the algorithmic complexity of the method scales linearly with respect to the number of particles thanks to the use of a modified Fast Multipole Method.

The current talk will present some results on the numerical analysis of this algorithm with a focus on proving that the method is indeed scalable with respect to the number of objects N in the problem. As a first step, we demonstrate that both the infinite-dimensional integral equation formulation and its Galerkin discretisation are well-posed with explicitly characterisable continuity and inf-sup constants. Our main result however is to derive error estimates and an

upper bound for the condition number of the stiffness matrix that do not explicitly depend on N . The first result establishes that for a fixed number of degrees of freedom, the error does not degrade as one increases the number of objects N . The second result helps establish that for a fixed number of degrees of freedom, a Krylov subspace solver such as GMRES converges to a given tolerance independent of N .

S18.05 | Numerical methods of differential equations

Date: February 20, 2019

16:30-18:30

Room: HS 31

A nonconforming Trefftz virtual element method for the fluid fluid interface problem

Lorenzo Mascotto (*Universität Wien, Austria*)

16:30

Alexander Pichler (*Universität Wien, Austria*)

We introduce a novel nonconforming Trefftz virtual element method based on general polygonal meshes for the approximation of solutions to a 2D fluid-fluid interface problem, i.e., to a Helmholtz problem with piecewise constant wave number. The local discrete spaces consist of plane and evanescent waves, plus additional functions defined implicitly as solutions to suitable local auxiliary Helmholtz problems. The degrees of freedom are associated with the mesh edges, and the global space is built in a nonconforming fashion (à la Crouzeix-Raviart). We present a variety of numerical experiments, including the h-, the p-, and the hp-versions of the method, employing both isotropic and anisotropic mesh refinements. The reason why the proposed approach can be considered as a very effective substitute to other well-established technologies tailored for the approximation of solutions to Helmholtz type problems, such as the plane wave discontinuous Galerkin method or the ultra-weak variational formulation, is that an orthogonalization-and-filtering technique, not applicable to the best of our knowledge in the discontinuous Galerkin setting, renders the nonconforming Trefftz virtual element approach particularly robust. More precisely, by eliminating "redundant" basis functions, it leads to a significant reduction of the number of the degrees of freedom and of the condition number of the system stemming from the method; in some occurrences, the method seems even to converge whilst keeping the dimension of the space almost fixed!

Resonance problems in waveguides with backward propagating modes

Lothar Nannen (*TU Wien, Austria*)

17:10

We consider time-harmonic linear elasticity equations in domains with waveguides. Since for such problems there exist modes with different signs of group and phase velocity, standard PML methods fail. We apply an infinite element method based on a pole condition, which characterizes outgoing solutions by the poles of their Laplace transform in propagation direction. Since this condition is frequency independent, it is well-suited for resonance problems. Moreover, numerical tests show super-algebraic convergence with respect to the number of unknowns in direction of wave propagation.

A beam propagation method for perturbed Gaussian beams

Christoph Pflaum (*Universität Erlangen Nürnberg, Germany*)

17:30

Perturbed Gaussian beams arise in several applications in optics. One of them is a laser amplifier. In a laser amplifier a Gaussian beam is distorted by thermal lensing effects, polarization effects and gain guiding. This leads to a decrease of the beam quality at the output of a laser amplifier. An important question is how to calculate this decrease of the beam quality and how to compute the amplified beam. There exist several difficulties of existing simulation techniques for the computation of optical beams. These are the high computational amount in order to resolve the phase of the beam and modelling non-absorbing boundary conditions. We present a new beam propagation method, which circumvents these difficulties. The idea is to decompose the beam as a product of a Gaussian Beam TEM00 and an unknown distortion function Φ . This leads to an interesting partial differential equation for Φ , which contains a beam spreading convection term. This PDE is solved numerically by finite elements and a Crank-Nicolson space stepping discretization. The resulting linear equation system is solved by GMRES. The q-parameter of the Gaussian beam is calculated in advance by an ABCD matrix method. This leads to a highly efficient simulation technique. It can be applied to simulate the amplification of Gaussian beams in laser amplifiers.

On the computation of localized Schrödinger eigenstates

Robert Altmann (*University of Augsburg, Germany*)

17:50

Daniel Peterseim (*University of Augsburg, Germany*)

We consider the linear Schrödinger operator with oscillatory high-amplitude potentials on bounded domains. The appearance of disorder in the potential then leads to a localization of the lowermost eigenstates. This means that these eigenstates decay exponentially, which can be proven using iterative solvers in combination with an optimal local preconditioning. In this talk we aim to apply these techniques also numerically in order to actually compute the first eigenstates of the linear Schrödinger operator. For this we apply methods used in numerical homogenization.

Localized Orthogonal Decomposition for the wave equation

Roland Maier (*University of Augsburg, Germany*)

18:10

Daniel Peterseim (*University of Augsburg, Germany*)

We consider the approximation of solutions to the wave equation in media with (spatial) micro-scale features. In such a setting, the classical finite element method requires very small mesh sizes in order to produce acceptable results and, thus, the computations become very expensive. To avoid this, we use numerical homogenization (Localized Orthogonal Decomposition method) to deal with the finescale features and to allow for computations on relatively coarse meshes. We prove optimal convergence rates and investigate the interplay between mesh sizes in space and time.

S18.06 | Numerical methods of differential equations

Date: February 20, 2019

16:30-18:30

Room: SR 08

hp-FEM for the spectral fractional Laplacian in polygons

Jens Markus Melenk (*TU Wien, Austria*)

16:30

Lehel Banjai (*TU Wien, Austria*)

Christoph Schwab (*TU Wien, Austria*)

For the spectral fractional Laplacian in polygons we present two types of discretizations that converge at an exponential rate. The first one is based on the Caffarelli-Silvestre extension, which realizes the non-local fractional Laplacian as a Dirichlet-to-Neumann map of a (degenerate) elliptic boundary value problem (BVP). This BVP is amenable to a discretization by high order finite element method (hp-FEM). Exponential convergence of the hp-FEM can be achieved if the underlying meshes are suitably refined towards the edges of the polygon so as to resolve the boundary singularities and towards the vertices in order to capture the corner singularities. The second discretization is based on the so-called Balakrishnan formula, an integral representation of the inverse of the spectral fractional Laplacian. The discretization of the integral leads to a collection of BVPs, which can be discretized by hp-FEM. Again, the use of meshes that are refined towards the vertices and the boundary leads to exponential convergence.

A reduced basis method for fractional diffusion operators

Tobias Danczul (*TU Wien, Austria*)

17:10

Joachim Schöberl (*TU Wien, Austria*)

Several authors have proposed and analyzed numerical methods for fractional differential operators, in particular Fourier Galerkin schemes and Caffarelli-Silvestre extensions.

By means of a reduced basis method, we project the operator to a low dimensional space, where the fractional power can be directly evaluated via the eigen-system. By an optimal choice of the sample points we can prove exponential convergence. Numerical experiments evaluating the operator and the inverse operator confirm the analysis.

Finally, we consider the time-dependent Fractional Cahn-Hilliard Equation (FCHE). By a splitting method we decouple the non-linear operator from the fractional diffusion operator. The linear fractional parabolic equation is solved on the low dimensional reduced basis space.

All proposed methods are easy to implement into existing finite element packages. In our case, the algorithms were implemented within the Python interface NGS-Py of the finite element library NGSolve.

Exponential convergence of an hp-FEM approximation for parabolic fractional diffusion

Alexander Rieder (*TU Wien, Austria*)

17:30

Jens Markus Melenk (*TU Wien, Austria*)

In this talk, we present an approximation scheme for the following time dependent fractional diffusion problem on a bounded domain.

$$u_t + (-\Delta)^s u = f, \quad u(0) = u_0, \quad \text{and} \quad u_{\partial\Omega} = 0$$

with a parameter $s \in (0, 1)$.

In order to localize the non-local operator $(-\Delta)^s$, we employ the so-called Caffarelli-Silvestre extension, which yields an equivalent $d + 1$ -dimensional local problem. This kind of problem exhibits two sources of singularities, which need to be taken into account for the numerical scheme: The extended problem is degenerate for $y \rightarrow 0$, where y is the extended variable, and for $t \rightarrow 0$, the parabolic problem may suffer from startup singularities due to incompatibilities of the data with the boundary condition on u . For discretization, we consider a hp -type finite element discretization in space, and an hp -DG method for the time variable. In the one dimensional setting (i.e., $d=1$), we rigorously prove exponential convergence of the method without imposing a compatibility condition on the data.

Numerical homogenization of heterogeneous fractional Laplacians

Donald L. Brown (*The Equity Engineering Group, USA*)

17:50

Joscha Gedicke (*University of Vienna, Austria*)

Daniel Peterseim (*University of Augsburg, Germany*)

In this talk, we develop a numerical multiscale method to solve the fractional Laplacian with a heterogeneous diffusion coefficient. When the coefficient is heterogeneous, this adds to the computational costs. Moreover, the fractional Laplacian is a non-local operator in its standard form, however the Caffarelli-Silvestre extension allows for a localization of the equations. This adds a complexity of an extra spacial dimension and a singular/degenerate coefficient depending on the fractional order. Using a sub-grid correction method, we correct the basis functions in a natural weighted Sobolev space and show that these corrections are able to be truncated to design a computationally efficient scheme with optimal convergence rates. A key ingredient of this method is the use of quasi-interpolation operators to construct the fine scale spaces. Since the solution of the extended problem on the critical boundary is of main interest, we construct a projective quasi-interpolation that has both d and $d+1$ dimensional averages over subsets in the spirit of the Scott-Zhang operator. We show that this operator satisfies local stability and local approximation properties in weighted Sobolev spaces. We further show that we can obtain a greater rate of convergence for sufficient smooth forces, and utilizing a global L^2 projection on the critical boundary. We present some numerical examples, utilizing our projective quasi-interpolation in dimension $2+1$ for analytic and heterogeneous cases to demonstrate the rates and effectiveness of the method.

Optimal adaptivity and preconditioning for the fractional Laplacian

Markus Faustmann (*TU Wien, Austria*)

18:10

Jens Markus Melenk (*TU Wien, Austria*)

Maryam Parvizi (*TU Wien, Austria*)

Dirk Praetorius (*TU Wien, Austria*)

We present novel inverse estimates for the (integral) fractional Laplacian. More precisely, we show that a weighted L^2 -norm, where the weight is a power of the local mesh-width, of the fractional Laplacian can be bounded by the energy norm. Generalizing the arguments used in the boundary element method, the non-local operator is split into a localized near-field and a smoother far-field part, which is treated using the so-called Caffarelli-Silvestre extension problem and interior regularity estimates. Weighted L^2 -norms appear naturally in the context of a posteriori error estimation in adaptive methods. With the help of our inverse estimate, we prove optimal convergence rates of an adaptive algorithm steered by a weighted residual error estimator. Moreover, we propose a different, reliable weighted error estimator to cover the open case of fractional powers larger than $3/4$. As a second application of the inverse inequalities,

we prove that an additive Schwarz preconditioner of BPX-type for the fractional Laplacian on locally refined meshes leads to condition numbers that are uniformly bounded in the refinement level.

S18.07 | Numerical methods of differential equations

Date: February 21, 2019
Room: HS 31

08:30-10:30

Multiscale methods for electromagnetic wave propagation in media with high contrast

Barbara Verfürth (*University of Augsburg, Germany*)

08:30

The propagation of electromagnetic fields in periodic materials is considered with growing interest as these media can show unusual behavior, such as frequency band gaps and even negative refraction. To produce such effects, the materials possess some (periodic) sub-wavelength fine-scale structures, which nevertheless come into resonance with the incident wave.

The simulation of such problems is quite challenging due to the general wave nature of the problem and the additional fine-scale oscillations from the material inhomogeneities. A direct numerical treatment with standard methods easily exceeds today's available computer resources. In this talk, we consider electromagnetic scattering problems with rapidly oscillating coefficients with high contrast. This leads to unusual effective coefficients in the homogenization limit for the periodic case.

Motivated by these results of homogenization, we introduce numerical multiscale methods to simulate the macroscopic behavior of the waves. Additional (fine-scale) correctors are needed to obtain good L^2 -approximations. In particular, we discuss how these correctors can be computed efficiently by solving only localized fine-scale problems.

Numerical experiments are presented to confirm our theoretical results and to gain an insight into some unusual optical phenomena.

Space-time methods for Maxwell's equations

Julia Ines Mareike Hauser (*Graz University of Technology, Austria*)

09:10

Olaf Steinbach (*Graz University of Technology, Austria*)

Maxwell's equations are the key to electro magnetic problems. There are many approaches to solve these equations. Most try to eliminate the time derivative to simplify the equations. In contrast to these methods our approach considers time as another dimension and looks at Maxwell's equations in a corresponding 4D space-time setting. For that purpose we look at the equations on a bounded Lipschitz domain in space and a bounded interval in time. The electric permittivity and magnetic permeability shall be symmetric, positive definite and bounded matrix functions. We will consider different variational formulations and determine under what conditions Maxwell's equations are uniquely solvable. In the end we take a look at numerical methods for these problems.

A hybrid WKB-based method for Schrödinger scattering problems in the semi-classical limit

Anton Arnold (*TU Wien, Austria*)

09:30

We are concerned with 1D scattering problems related to quantum transport in (tunneling) diodes. The problem includes both oscillatory and evanescent regimes, partly including turning points. We shall discuss the efficient numerical integration of ODEs of the form $\epsilon^2 u'' + a(x)u = 0$ for $0 < \epsilon \ll 1$ on coarse grids, but still yielding accurate solutions. In particular we study the numerical coupling of the highly oscillatory regime (i.e. for given $a(x) > 0$) with evanescent regions (i.e. for $a(x) < 0$). In the oscillatory case we use a marching method that is based on an analytic WKB-preprocessing of the equation. And in the evanescent case we use a FEM with WKB-ansatz functions.

We present a full convergence analysis of the coupled method, showing that the error is uniform in epsilon and second order w.r.t. h , when $h = O(\epsilon^{1/2})$. We illustrate the results with numerical examples for scattering problems for a quantum-tunnelling structure.

The main challenge when including a turning point is that the solution gets unbounded there as $\epsilon \rightarrow 0$. Still one can obtain epsilon-uniform convergence, when $h = O(\epsilon^{7/12})$.

The talk is based on joint work with Claudia Negulescu; Kirian Döpfner.

References:

* A. Arnold, K. Döpfner: Stationary Schrödinger equation in the semi-classical limit: WKB-based scheme coupled to a turning point, submitted 2018

* A. Arnold, C. Negulescu: Stationary Schrödinger equation in the semi-classical limit: numerical coupling of oscillatory and evanescent regions, *Numerische Mathematik* 138, No. 2 (2018) 501-536

* A. Arnold, N. Ben Abdallah, C. Negulescu: WKB-based schemes for the oscillatory 1D Schrödinger equation in the semi-classical limit, *SIAM J. Numer. Anal.* 49, No. 4 (2011) 1436-1460

Inf-sup stable space-time variational formulations for the second order wave equation

Marco Zank (*TU Graz, Austria*)

09:50

Olaf Steinbach (*TU Graz, Austria*)

For the discretisation of time-dependent partial differential equations usually explicit or implicit time stepping schemes are used. An alternative approach is the usage of space-time methods, where the space-time domain is discretised and the resulting global linear system is solved at once. In any case the underlying space-time variational formulation plays a decisive role for space-time Galerkin methods. In this talk for the scalar wave equation variational formulations which are well-suited for space-time Galerkin methods are investigated. First, a brief overview of known results about variational formulations for the wave equation is presented. Second, two space-time approaches for the second order wave equation are introduced. Uniqueness and existence including corresponding inf-sup conditions are proven. In both cases the starting point is a Hilbert space H and then the idea is to use a completion procedure to define a subspace H_0 of H where a Poincaré-Friedrichs type inequality holds. This idea leads to a uniquely solvable variational formulation in H_0 . In the first approach the second order wave equation is considered in the sense of L^2 , whereas in the second one a weaker sense than L^2 is examined. Finally, examples for solutions of the wave equation are presented and discussed.

S18.08 | Numerical methods of differential equations

Date: February 21, 2019

08:30-10:30

Room: SR 08

Differentiable mappings for finite element meshes

Daniel Arndt (*Universität Heidelberg, Germany*)

08:30

Guido Kanschat (*Universität Heidelberg, Germany*)

Finite element methods of higher continuity, for instance H^2 -conforming for biharmonic problems or H^1 -conforming elements with matching pressure space for the Stokes problem, require mappings from the reference cell which are at least C^1 across element boundaries. We discuss the construction of the lowest order version of such mappings for quadrilateral and hexahedral meshes and their implementation in the general purpose finite element code deal.II

A second order multipoint flux mixed finite element method on hybrid meshes

Bogdan Radu (*TU Darmstadt, Germany*)

08:50

Herbert Egger (*TU Darmstadt, Germany*)

We consider the numerical approximation of subsurface flow problems by a mixed finite element method. Following ideas of Wheeler and Yotov, we utilize a mass-lumping strategy that allows us to circumvent the saddle point structure of the underlying variational problem by local elimination of the flux variables leading to a Poisson-type problem for the pressure only. An abstract convergence analysis is given, which allows us to obtain second order approximations on hybrid meshes. We further show that even third order convergence for the pressure can be obtained by local postprocessing. The theoretical results will be illustrated by numerical tests which demonstrate the efficiency of the method.

Acknowledgement. This work is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

Anisotropic mesh adaptation: from crack propagation to topology optimization

Nicola Ferro (*Politecnico di Milano, Italy*)

09:10

Stefano Micheletti (*Politecnico di Milano, Italy*)

Simona Perotto (*Politecnico di Milano, Italy*)

Mesh adaptation is a widely employed technique to select the computational mesh most suited for the problem at hand, i.e., the grid characterized by fine elements where the solution exhibits irregularities (such as boundary or internal layers, shocks, singularities), and coarse triangles where the solution is smooth. We can mainly distinguish between isotropic and anisotropic meshes. In the isotropic case, the adapted mesh is generated by tuning the size of the elements only. On the contrary, when dealing with anisotropic meshes, we can select not only the size but also the shape and the orientation of the triangles in order to follow the intrinsic directionalities of the solution. This guarantees a considerable reduction of the number of elements required to ensure a desired accuracy on a discretization of the considered problem.

This presentation focuses on anisotropic meshes. In particular, we refer to the anisotropic setting used, for instance, in [1,2], where the generation of the adapted grid is driven by an anisotropic a posteriori error analysis. In particular, we focus on two settings where anisotropic mesh

adaptation may have a significant impact, namely fracture evolution in brittle materials and structural optimization.

The crack tracking is modeled by minimizing the Ambrosio-Tortorelli energy functional, in combination with an anisotropic mesh adaptation procedure. A very sharp detection of the crack path is thus possible, by employing a contained number of (locally very stretched) triangles [3]. Concerning the design of structures, we resort to both shape and topology optimization. A standard geometric approach is used for shape optimization, while the density-based SIMP method, enriched with the employment of anisotropic adapted meshes [4], is adopted to set the new layout of the structure. The resulting configurations present innovative shapes and are extremely smooth, thus demanding a contained post-processing before moving to manufacturing.

References

- [1] L. Formaggia, S. Micheletti, S. Perotto. "Anisotropic mesh adaptation with application to CFD problems", Proceedings of WCCM V, Fifth World Congress on Computational Mechanics, 2002.
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- [3] M. Artina, M. Fornasier, S. Micheletti, S. Perotto, "Anisotropic mesh adaptation for crack detection in brittle materials". Siam Journal on Scientific Computing, 2015.
- [4] S. Micheletti, S. Perotto, L. Soli. "Adaptive Topology Optimization for Additive Layer Manufacturing", Patent application.

Two-grid hp-version DGFEM for second-order quasilinear elliptic PDEs with agglomerated coarse meshes

Scott Congreve (*University of Vienna, Austria*)

09:30

Paul Houston (*University of Nottingham, UK*)

In this talk, we consider the extension of so-called two-grid hp-version discontinuous Galerkin finite element methods (DGFEM) for the numerical solution of a second-order quasilinear elliptic boundary value problem of monotone type to the situation of using agglomerated polygonal/polyhedral meshes for the coarse mesh approximation. Two-grid methods first approximate an underlying nonlinear problem on a coarse finite element partition of the computational domain and then on the basis of this coarse grid approximation compute a linearized variant of the discrete problem on a finer mesh.

Previous work has studied the a priori and a posteriori error analysis for the hp-version DGFEM for strongly monotone quasilinear PDEs on meshes of simplices, quadrilaterals, and hexahedra. Here, we consider the extension of this analysis to a two-grid method where the coarse mesh solution is obtained by solving a DGFEM on a mesh consisting of general polygonal/polyhedral elements constructed by agglomerating a fine mesh of simplices, quadrilaterals, or hexahedra. Moreover, we extend the existing hp-adaptive two-grid algorithm to adaptively designing the coarse finite element space for agglomerated elements. Numerical experiments are presented for two- and three-dimensional problems to demonstrate the computational improvement of the hp-adaptive two-grid method, when compared to the standard discontinuous Galerkin method.

Symbolic evaluation of hp-FEM element matrices on simplices

Tim Haubold (*Leibniz University Hannover, Germany*)

09:50

In this talk we consider high-order finite element discretizations of linear elliptic boundary value problems. Following e.g. [Beuchler et al., 2012 [1], Karniadakis, Sherwin (1999) [2]] a set of hierarchic basis functions on simplices is chosen. For an affine simplicial triangulation this leads to a sparse stiffness matrix. Moreover the L^2 -inner product of the interior basis functions is sparse with respect to the polynomial order \mathbf{p} . The construction relies on a tensor-product based

construction with properly weighted Jacobi polynomials. In this talk we present algorithms which compute the remaining non zero entries of mass- and stiffness matrix in optimal arithmetical complexity. In order to obtain this result, recursion formulas based on symbolic methods are used. [3] The presented techniques can be applied not only to scalar elliptic problems in \mathbf{H}^1 but also for vector valued problems in $\mathbf{H}(\text{div})$ and $\mathbf{H}(\text{curl})$, where an explicit splitting of the higher-order basic functions into solenoidal and non-solenoidal ones is used.

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[3] Kauers: SumCracker - A Package for Manipulating Symbolic Sums and Related Objects, (2006)

Mixed explicit implicit schemes for embedded boundary geometries

Sandra May (*TU Dortmund University, Germany*)

10:10

Marsha Berger (*New York University, United States*)

Fabian Laakmann (*Oxford University, England*)

For flow simulations in complex geometry, the use of cut cell meshes is typically cheaper and faster than employing body-fitted grids. In this approach the geometry is simply cut out of a Cartesian background grid. This results in so called 'cut cells' around the boundary of the embedded object. These cells have irregular shape and may be very small. In the context of solving time-dependent, hyperbolic partial differential equations, probably the biggest issue caused by this approach is the so called 'small cell problem' - explicit time stepping schemes are not stable on the arbitrarily small cut cells. We present mixed explicit implicit finite volume schemes to overcome this problem. For simplicity, we focus on solving the time-dependent advection equation. We use an implicit timestepping scheme near the embedded boundary for stability; and employ an explicit scheme otherwise to keep the cost low. We combine the explicit and implicit scheme by means of 'flux bounding' - this way of coupling preserves mass conservation and ensures stability in form of a TVD result [1]. In this talk, we focus on the accuracy of the mixed scheme. One essential source of error is the transitioning from one timestepping scheme to the other. We will discuss how these errors accumulate and how to avoid their accumulation. We will present numerical results in one and two dimensions to support our theoretical findings.

[1] S. May, M. Berger, An explicit implicit scheme for cut cells in embedded boundary meshes, J. Sci. Comput., Vol. 71, pp. 919-943, 2017.

S18.09 | Numerical methods of differential equations

Date: February 21, 2019

14:00-16:00

Room: HS 31

Finite element approximation of second order PDEs in non-divergence form

Jan Blechschmidt (*TU Chemnitz, Germany*)

14:00

Roland Herzog (*TU Chemnitz, Germany*)

Max Winkler (*TU Chemnitz, Germany*)

Considered are second-order partial differential equations in a non-divergence form

$$A : D^2(u) = f \quad \text{in } \Omega$$

in some bounded domain planar domain Ω . These kind of equations typically arise as subproblems for the solution of Hamilton-Jacobi-Bellman equations in the context of stochastic optimal

control or when linearizing of fully non-linear second-order PDE, for instance the Monge-Ampere equation. Usually, the coefficients of A are non-differentiable in these applications and thus, the equations must be treated directly in a non-variational form. We investigate a non-conforming finite element approximation of these problems using higher-order Lagrange-elements for the approximation of u and continuous or discontinuous elements for some discrete Hessian. Of particular interest are a priori and a posteriori error estimates.

On the benefits of divergence-conforming (Hybrid) DG FEM for incompressible flows

Philip Lukas Lederer (*Vienna University of Technology, Austria*)

14:20

Christoph Lehrenfeld (*University of Goettingen, Germany*)

Gert Lube (*University of Goettingen, Germany*)

Joachim Schöberl (*Vienna University of Technology, Austria*)

Philipp W. Schroeder (*University of Goettingen, Germany*)

In this talk we consider divergence-conforming discretizations of the unsteady incompressible Navier-Stokes equations in a velocity-pressure formulation and present benefits of divergence-conforming schemes and tools to make them efficiently computable.

The result of a divergence-conforming discretization is a discretely exactly divergence-free velocity solutions which has the following important advantages:

- Conservation properties (kinetic energy, linear/angular momentum) for the unsteady incompressible Navier-Stokes equations. This implies energy-stability of a semi-discretization,
- Re-semi-robustness, i.e. error estimates for the unsteady incompressible Navier-Stokes equations that do not explicitly depend on the Re number,
- pressure robustness, i.e. discrete velocity errors that are independent of the pressure approximation.

The use of divergence-conforming schemes requires a weak imposition of tangential continuity by a DG or Hybrid DG scheme. We discuss several tools to compensate for the increased computational overhead of these schemes:

- Operator splitting time integration
- Hybridization with reduced stabilization ("projected jumps")
- Relaxed $H(\text{div})$ -conforming finite element spaces for superconvergence
- High order divergence-free basis functions

Finally, we present numerical examples and discuss the performance for 2D and 3D laminar and underresolved turbulent flows.

The Mass Conserving Mixed Stress (MCS) method for the Stokes equations: recent developments

Philip Lukas Lederer (*TU Wien, Austria*)

14:40

Joachim Schöberl (*TU Wien, Austria*)

Jay Gopalakrishnan (*Portland State University, USA*)

One of the main difficulties in computational fluid dynamics lies in the proper treatment of the incompressibility condition. A weak treatment of this constraint can lead to a locking phenomena if the viscosity is small and results in bad velocity approximations. Recent developments show that $H(\text{div})$ -conforming finite elements for the approximation of the velocity provide major benefits such as exact mass conservation, pressure-independent (locking free) and polynomial robust error estimates.

The Mass Conserving Mixed Stress (MCS) method for the Stokes equations is based on introducing a new variable which approximates the gradient of an $H(\text{div})$ -conforming velocity. For the analysis a new function space, the $H(\text{curldiv})$, is defined, in which we can show well posedness. We present the construction of proper Finite elements and discuss solvability.

Recent development show that also the symmetric gradient of the velocity can be approximated in a weak sense. We verify our method with several numerical examples implemented in NGSolve (www.ngsolve.org) with the new NGS-Py interface.

A locally weighted least-squares finite element method for the advection-reaction equation

Steffen Muenzenmaier (*University of Duisburg-Essen, Germany*)

15:00

Tom Manteuffel (*University of Colorado Boulder, USA*)

Ben Southworth (*University of Colorado Boulder, USA*)

This talk examines the first-order system least squares method for the transport (or reaction-advection) equation. A general Boltzmann transport equation, which describes the transport of neutral particles through a material media, can be efficiently solved by the the Discrete Ordinates Method (DOM) and Diffusion Synthetic Acceleration (DSA). The dominant computational expense in such a method is performing "transport sweeps", which consist of solving the transport equation for many different angles. These transport sweeps can be solved for example by (lumped) corner balance, SUPG or (upwinded) discontinuous Galerkin methods. Another approach undertaken in the transport community is the so called self-adjoint form, which corresponds to a least-squares finite element method and will be examined in this talk.

The focus of this talk is on problems where the total cross-sections may differ by several orders of magnitude across the spatial domain. When using least squares finite element methods, a naive approach can lead to unphysical behavior, such as unphysical damping, flux-dips, and cross-stream diffusion, requiring excessively fine grids to get a reasonable solution. The first part of this talk examines how these problems can be overcome by applying a proper local scaling to the problem. This can greatly increase the accuracy of the discrete solution without introducing any significant additional computational cost. In the second part of the talk, an efficient AMG-solver for the resulting linear equation systems is presented. The dependence on the scalings introduced earlier with respect to accuracy per cost is closely examined and adaptive refinement strategies are investigated.

Solving compressible Navier-Stokes equations on simplex space-time meshes

Max von Danwitz (*RWTH Aachen University, Germany*)

15:20

Violeta Karyofylli (*RWTH Aachen University, Germany*)

Norbert Hosters (*RWTH Aachen University, Germany*)

Marek Behr (*RWTH Aachen University, Germany*)

Simultaneously discretizing space and time with simplex finite elements extends the flexibility of unstructured meshes from space to space-time, allowing, e.g., local temporal refinement. A robust method to generate 4D simplex meshes proposed in [1] was used in [2] to compute incompressible two-phase flows in engineering geometries. In this contribution, we combine the SUPG stabilized

finite element formulation for compressible flows of [3] with simplex space-time meshes. The resulting discretizations are continuous in space, but discontinuous at distinct time levels. The potential of the resulting method is harnessed in flow simulations of seals and valves. 4D time refinement allows to adjust the resolution in the space-time mesh to the local flow conditions. Resulting computation time savings are shown for a three-dimensional transient simulation of blow-by past piston rings. Unstructured space-time meshes also enable flow simulations on spatial domains that change topology with time. We demonstrate this with a two-dimensional simulation of compressible flow in a valve that closes and opens. To be able to simulate problems of engineering interest, it is necessary to parallelize the computations. We present a way to enable parallel in time computations with simplex space-time meshes. In particular, the influence of space-time domain-decomposition on the performance of the employed GMRES and Newton-Raphson solver is investigated.

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- [3] Fei Xu, George Moutsanidis, David Kamensky, Ming-Chen Hsu, Muthuvel Murugan, Anindya Ghoshal, and Yuri Bazilevs, “Compressible flows on moving domains: Stabilized methods, weakly enforced essential boundary conditions, sliding interfaces, and application to gas-turbine modeling”, *Computers & Fluids*, 158 (2017) 201-220.

Efficient numerical methods for solving optimal control problems

Petra Csomós (*Eötvös Loránd University, Hungary*)

15:40

Optimal control problems are used to determine the suitable way how to drive a system into its predefined state, meanwhile certain optimality criterion is fulfilled. Latter is usually achieved by minimizing a cost functional being a function of the state and the control function. The optimal state is then obtained from a differential equation incorporating the operator, which corresponds to the dynamics, and the optimal control function resulting from the minimization. A special case is the linear quadratic regulator (LQR) problem with linear operators for the dynamics and the control, and a quadratic continuous-time cost functional.

In the talk we consider the numerical approximation to LQR problems for partial differential equations where the dynamics is driven by a strongly continuous semigroup. We present two approaches based on (i) operator splitting and (ii) exponential integrator idea. Both approaches treat the dynamics and the control separately. Furthermore, Fourier’s method allows the fast and accurate approximation of the effect of the dynamics (the operator semigroup) making our approach computationally efficient. We present the convergence’s proof for both approximation ideas, also in the case when certain spatial discretization methods are applied.

As an example, we illustrate our results with the shallow water equations being a special case of Navier–Stokes equations for incompressible and inviscid fluids moving on a rotating planet. These equations played an important role in the first attempts to describe the atmosphere’s large-scale dynamics. Numerical weather prediction models and ocean dynamical models, e.g. tsunami forecasting, are still based on them.

Since both approximation ideas rely on the generator property of the corresponding linear spatial differential operator, we first prove it for the linearized shallow water equations. Then we present the results of our numerical experiments when applying traditional discretization methods with and without operator splitting or exponential integrator. They clearly show the overperformance of our approach. At the end of the talk we present some animations.

The talk is partially based on the joint works with J. Winckler and H. Mena.

S18.10 | Numerical methods of differential equations

Date: February 21, 2019

14:00-16:00

Room: SR 08

A phase-field model for fractures in incompressible solids

Katrin Mang (*Leibniz Universität Hannover, Germany*)

14:00

Thomas Wick (*Leibniz Universität Hannover, Germany*)

Winnifried Wollner (*Technische Universität Darmstadt, Germany*)

In this talk, a quasi-static phase-field fracture model in incompressible solids is developed. Due to the incompressible material behavior, we derive a mixed system for the solid displacement equation resulting in two unknowns: a displacement field and a hydrostatic pressure variable. The fracture path is described with a phase-field function that is a smoothed indicator variable. Hence, the final system consists of three variables. In order to fulfill the stability of inf-sup type on the discrete level, we employ a Taylor-Hood element for the displacement-pressure system. The phase-field variable is spatially discretized with bilinear functions. The resulting discrete system is treated in a monolithic way and solved with a Newton-type method. Different numerical tests substantiate our model and algorithmic developments. These tests include spatial mesh refinement studies and variations in Poisson's ratio approaching the incompressible limit. Possible applications include to understand the fracture mechanism of incompressible materials such as rubber products.

Parameter-robust multigrid preconditioner for linear poroelastic media

Stefan Meggendorfer (*Heidelberg University, Germany*)

14:20

Guido Kanschat (*Heidelberg University, Germany*)

Biot's consolidation model is widely used for linear problems in poroelasticity. Recently, locking-free discretizations, robust with respect to incompressibility of fluid and solid and the Biot-Willis constant have been proposed. Since these discretizations result in large saddle-point systems, ill-conditioned with respect to standard finite element bases, effective preconditioners are needed for their iterative solution. We present a numerical study of a geometric multigrid preconditioner for strongly mass conservative $H(\text{div})$ -conforming finite element discretizations of Biot's linear consolidation model. Smoothers of overlapping Schwarz type are discussed and robustness with respect to the material parameters is achieved. In addition the method remains efficient for high order finite elements.

Stress reconstruction for elasticity problems

Fleurianne Bertrand (*Humboldt Universität zu Berlin, Germany*)

14:40

Bernhard Kober (*Humboldt Universität zu Berlin, Germany*)

Marcel Moldenhauer (*Humboldt Universität zu Berlin, Germany*)

Gerhard Starke (*Humboldt Universität zu Berlin, Germany*)

In this talk, a stress reconstruction in the $H(\text{div})$ -conforming Raviart-Thomas space based on the Taylor-Hood displacement-pressure approximation procedure for linear elasticity is proposed. The construction is weakly symmetric and the computation is performed locally on a set of vertex patches. Due to the weak symmetry constraint, the local problems need to satisfy consistency conditions associated with all rigid body modes. The resulting error estimator constitutes a guaranteed upper bound for the error and is shown to be local efficient.

Reconstruction-based a-posteriori error estimation in stress-based FEM for frictional contact problems

Bernhard Kober (*Universität Duisburg-Essen, Germany*)

15:00

Rolf Krause (*Università della Svizzera italiana, Italy*)

Gabriele Rovi (*Università della Svizzera italiana, Italy*)

Gerhard Starke (*Universität Duisburg-Essen, Germany*)

The use of stress-based finite element methods for the treatment of contact problems admits locking free performance in the incompressible limit as well as direct access to the surface forces at the contact zone. Consequently we are studying the application of the stress-based FEM described in [1] featuring next-to-lowest order Raviart-Thomas-Elements to the Signorini contact problem with Coulomb friction using a dual variational formulation similar to the one studied in [2].

Since frictional contact problems tend to feature singularities, adaptive refinement strategies are to be considered and reliable a-posteriori error estimation is needed. We therefore extend the a-posteriori error estimator in [5] to frictional contact and reconstruct a H^1 -conforming displacement following the ideas in [3] and [4]. We prove reliability of our error estimator under similar assumptions as those made in [6] for uniqueness and test its efficiency by numerical experiments.

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Symmetry breaking patterns in the numerical minimization of the elastic energy of thin films

Georg-Alexis Papathanassopoulos (*Albert-Ludwigs-Universität Freiburg, Germany*)

15:20

Sören Bartels (*Albert-Ludwigs-Universität Freiburg, Germany*)

We present a numerical scheme for the minimization of an Föppl-von Karman energy functional describing the bending, membrane and substrate energy of a thin film that is bonded to a large substrate. In compressing the substrate, experiments show, that the film tends to wrinkle or buckle if delamination is prohibited. Previous analysis gives a hint about the patterns related to the optimal energy scaling law in specific parameter regimes. There it is expected that so-called herringbone structures appear. Our numerical results confirm this theory.

Weakly symmetric stress reconstruction and a posteriori error estimation for hyperelasticity

Fleurianne Bertrand (*University of Duisburg-Essen, Germany*)

15:40

Bernhard Kober (*University of Duisburg-Essen, Germany*)

Marcel Moldenhauer (*University of Duisburg-Essen, Germany*)

Gerhard Starke (*University of Duisburg-Essen, Germany*)

By extending the techniques in [1] for the linear elastic case, an algorithm to reconstruct a $H(\text{div})$ -conforming weakly symmetric stress tensor for the non-linear hyperelastic case is presented. This work builds upon [2] where a local weakly symmetric stress reconstruction is derived for arbitrary conforming finite elements in linear elasticity. The reconstructed stress tensor is used as an a posteriori error estimator. Numerical results for the incompressible hyperelastic case are presented.

[1] F. Bertrand, M. Moldenhauer, G. Starke, A posteriori error estimation for planar linear elasticity by stress reconstruction, *Computational Methods in Applied Mathematics* (2018), <https://doi.org/10.1515/cmam-2018-0004>

[2] F. Bertrand, B. Kober, M. Moldenhauer, G. Starke, Weakly symmetric stress equilibration and a posteriori error estimation for linear elasticity, in review, available at: <https://arxiv.org/abs/1808.02655>

S18.11 | Numerical methods of differential equations

Date: February 21, 2019

17:40-18:40

Room: HS 31

Mode-based derivation of adjoint equations - a lazy man's approach

Julius Reiss (*TU Berlin, Germany*)

17:40

Mathias Lemke (*TU Berlin, Germany*)

Jörn Sesterhenn (*TU Berlin, Germany*)

A method to calculate the adjoint solution for a large class of partial differential equations is discussed. It differs from the known continuous and discrete adjoint, including automatic differentiation. Thus, it represents an alternative, third method.

It is based on a modal representation of the linearized operator of the governing (primal) system. To approximate the operator an extended version of the Arnoldi factorization, the dynamical Arnoldi method (DAM) is introduced. The DAM allows to derive approximations for operators of non-symmetric coupled equations, which are inaccessible by the classical Arnoldi factorization. The approach is applied to the Burgers equation and to the Euler equations on periodic and non-periodic domains.

Finally, it is tested on an optimization problem.

On some discrete boundary value problems for elliptic equations

Vladimir Vasilyev (*Belgorod National Research University, Russian Federation*)

18:00

Alexander Vasilyev (*Belgorod National Research University, Russian Federation*)

Oksana Tarasova (*Belgorod National Research University, Russian Federation*)

We consider a pseudo-differential operator with a symbol satisfying the strong ellipticity condition and study the Dirichlet problem assuming that there is unique solution for the boundary value problem in appropriate Sobolev-Slobodetskii spaces.

For approximate solution of the problem we construct a certain digital pseudo-differential operator acting in some discrete spaces [1, 2]. Further we introduce the corresponding discrete boundary condition and prove the solvability for the discrete boundary value problem.

Also we obtain some comparison results between discrete and continuous cases.

References

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S18.12 | Numerical methods of differential equations

Date: February 22, 2019

08:30-10:30

Room: HS 31

Space-time finite and boundary element methods

Olaf Steinbach (*TU Graz, Austria*)

08:30

In this talk I will give an overview on space time finite and boundary element methods for time-dependent problems with a particular focus on the heat equation. We will discuss and analyse several variational formulations and we will provide related numerical examples.

Parallel space-time finite element solvers of parabolic initial-boundary value problems with non-smooth solutions

Andreas Schafelner (*JKU Linz, Austria*)

09:10

Ulrich Langer (*JKU Linz, Austria*)

We consider locally stabilized, conforming finite element schemes on completely unstructured simplicial space-time meshes for the numerical solution of parabolic initial-boundary value problems with variable, possibly discontinuous in space and time coefficients. Discontinuous coefficients, non-smooth boundaries, changing boundary conditions, non-smooth or incompatible initial conditions, and non-smooth right-hand sides can lead to non-smooth solutions. For instance, in electromagnetics, permanent magnets cause line-delta-distributions in the source term in 2D quasi-magnetostatic simulations of electrical machines.

We present new a priori estimates for low-regularity solutions. In order to avoid reduced convergence rates appearing in the case of uniform mesh refinement, we also consider adaptive refinement procedures based on residual a posteriori error indicators. The huge system of space-time finite element equations is then solved by means of GMRES preconditioned by algebraic multigrid. In particular, in the 4D space-time case that is 3D in space, simultaneous space-time parallelization can considerably reduce the computational time.

The authors would like to thank the Austrian Science Fund (FWF) for the financial support under the grants NFN W1214-04.

Higher-order time stepping for micromagnetism

Michael Feischl (*University of Bonn, Germany*)

09:30

For the Landau-Lifshitz-Gilbert (LLG) equation of micromagnetics, we study linearly implicit backward difference formula (BDF) time discretizations up to order 5 combined with finite element space discretization based on a formulation due to Alouges. We prove stability and optimal-order error bounds in the situation of a sufficiently regular solution. For the BDF methods of orders 3 to 5, this requires that the damping parameter in the LLG equations be not too small, and in addition a mild time step restriction is required that is not needed for the A-stable methods of orders 1 and 2.

A new domain-based implicit-explicit time stepping scheme based on the class of exponential integrators called sEPIRK

Veronika Straub (*University of Kassel, Germany*)

09:50

Sigrun Ortleb (*University of Kassel, Germany*)

Andreas Meister (*University of Kassel, Germany*)

Philipp Birken (*Lund University, Sweden*)

The simulation of flows around complex geometries or similar applications often inherit the task of solving large, stiff systems of ODEs. Domain-based implicit-explicit (IMEX) type schemes offer the possibility to apply two different time integration schemes - e.g. an explicit and an implicit one - to different parts of the computational domain. The goal hereby is to decrease the computational cost by lessening the CFL restriction on the maximum stable time step size by excluding the smallest elements from the explicit time stepping method on the one hand, and by reducing the system sizes of the nonlinear and linear systems of the implicit scheme on the other hand.

We adopt the recently introduced exponential integrators called sEPIRK by Rainwater and Tokman (2014) in the domain-based IMEX setting and call them IMEX-sEPIRK schemes. This type of schemes stand out by solving the linear part of the ODE exactly while evaluating the matrix-exponential like functions in an efficient way utilizing the adaptive Krylov subspace approximation algorithm documented by Niesen and Wright (2012). That leads to A-stability, which is a desired property of an implicit scheme. Thus, our aim is to apply the exponential integrator within the sEPIRK scheme to the implicit part of the computational domain, whereas the explicit part of the scheme, which turns out to be a Runge-Kutta scheme, is applied to the explicit part of the domain.

In our earlier research we have shown that additive coupling of the EPIRK and sEPIRK schemes with (explicit) Runge-Kutta schemes yield schemes of at most first order of convergence. With the IMEX-sEPIRK schemes we now found a way to exploit exponential integrators in the domain-based IMEX setting without a limitation of the convergence order. We compare third order IMEX-sEPIRK schemes to the IMEX-Runge-Kutta schemes applied in the context of discretized PDEs by Kanevsky, Carpenter, Gottlieb and Hesthaven (2007).

First, we verify the experimental order of convergence of the third order IMEX-sEPIRK schemes for the 2D Shu-Vortex test case based on the Euler equations discretized by the Discontinuous Galerkin approach. Next, we analyze the efficiency gain in comparison with non-IMEX schemes for geometry-induced stiffness for the 1D viscous Burgers equation discretized by the Finite Difference method in space. And finally, we perform the computation of a steady state flow around the cross section of an airfoil with the new schemes.

Numerical integration of coupled problems via convolution quadrature

Vsevolod Shashkov (*TU Darmstadt, Germany*)

10:10

Herbert Egger (*TU Darmstadt, Germany*)

Kersten Schmidt (*TU Darmstadt, Germany*)

We consider the numerical solution of coupled linear-nonlinear differential algebraic systems under the assumption that the size of the system is dominated by the linear part which may, e.g., stem from semi-discretization of a partial differential equation. Using linearity, the linear subproblem can be eliminated in frequency domain which leads to an integro-differential algebraic equation for the variable of the small nonlinear subsystem only. For the solution of this reduced problem, we consider single- and multistep methods together with a convolution quadrature for the integral terms. We show that an appropriate choice of the time-stepping and convolution quadrature schemes yields a method that can be interpreted as a standard numerical approximation of the original coupled problem which automatically ensures stability and accuracy of the method. After a computationally expensive pre-processing step in which the weights for the convolution quadrature are computed, the time integration of the system can then essentially be realized at the complexity of the small nonlinear sub-problem. The reliability and efficiency of the method will be demonstrated by numerical examples.

S19 | Optimization of differential equations

Organiser: Kathrin Welker (*Trier University, Germany*)
Winnifried Wollner (*Technische Universität Darmstadt, Germany*)

S19.01 | Optimization of differential equations

Date: February 19, 2019 08:30-10:30
Room: HS 30

An optimal design of an elastic plate in a dynamic contact with a rigid obstacle

Igor Bock (*FEI Slovak University of Technology, Slovak Republic*) 08:30
Mária Kečkemétyová (*FEI Slovak University of Technology, Slovak Republic*)

We deal with an optimal control problem governed by a nonlinear hyperbolic initial-boundary value problem describing the perpendicular vibrations of a simply supported anisotropic elastic plate against a rigid obstacle. A variable thickness of a plate plays the role of a control variable. We verify the existence of an optimal thickness function and derive necessary optimality conditions. The state initial-boundary value problem will be solved by the penalization method. We have solved a similar problem for a short memory viscoelastic plate in [1]. There is no uniqueness and less regularity of a solution in the elastic case. The second time derivative expressing the acceleration of vibrations is expressed as a vector measure (see [2]). We solve the regularized optimal control problem with a state penalized equation firstly. As the original state variables serve solutions of the original variational inequality received as limits of solutions to penalized problems. The optimal thickness function corresponding to the original state variational inequality can be obtained as the limit of a sequence of optimal thicknesses solving the regularized problems. The necessary optimality conditions have the generalized character. They will be received using the necessary optimality conditions connected with the penalized state problem. We remark that solving the dynamic contact problem for an elastic membrane vibrating against a rigid obstacle is still an open problem.

Acknowledgement. The work presented here is supported by the Ministry of Education of Slovak Republic under VEGA grant 1/0819/17.

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Necessary optimality conditions of VI constrained shape optimization problems

Kathrin Welker (*HSU/UniBw Hamburg, Germany*) 08:50
Daniel Luft (*Trier University, Germany*)
Volker Schulz (*Trier University, Germany*)

In this talk, shape optimization problems constrained by variational inequalities (VI) are treated from an analytical and numerical point of view in order to formulate approaches aiming at semi-smooth Newton methods on shape spaces. In contrast to classical VIs, where no explicit dependence on the domain is given, VI constrained shape optimization problems are in particular highly challenging because of the two main reasons: Firstly, one needs to operate in inherently non-linear, non-convex and infinite-dimensional shape spaces. Secondly, one cannot expect for

an arbitrary shape functional depending on solutions to VIs the existence of the shape derivative or to obtain the shape derivative as a linear mapping, which imply that the adjoint state cannot be introduced and, thus, the problem cannot be solved directly without any regularization techniques. In this talk, we investigate analytically a VI constrained shape optimization problem with respect to its first-order necessary optimality conditions. The analytical insight in this problem enables its computational treatment which is also presented in this talk.

Efficient interface identification with an optimum experimental design

Martin Siebenborn (*Universität Hamburg, Germany*)

09:10

In many applications, which are modeled by partial differential equations, there is a small number of spatially distributed materials or parameters distinguished by interfaces. It is thus preferable to treat the shape as variable instead of the parameter itself in order to achieve high spatial resolutions. The identification of these interfaces leads to infinite dimensional optimization problems since shapes are typically interpreted as points on a manifold. In this talk we present an optimum experimental design approach for this class of shape optimization problems. Starting from an algorithm for the interface identification in diffusion processes we develop a method which describes optimal sensor placements in space and time. In particular, we comment on the challenges arising compared to classical OED in vector spaces.

Here we encounter a parameter identification problem in which the parameter space bears the structure of a shape manifold. The goal is to improve the estimation precision within a certain subspace of the infinite dimensional tangent space, and to find those shape variations of best and worst identifiability.

A discrete shape manifold and its use in PDE-constrained shape optimization

Ronny Bergmann (*Chemnitz University of Technology, Germany*)

09:30

Roland Herzog (*Chemnitz University of Technology, Germany*)

Estefania Loayza-Romero (*Chemnitz University of Technology, Germany*)

A shape can be defined in various ways, as plane curves, characteristic functions of measurable sets, surfaces in higher dimensions, boundary contours of objects or images, and as the most simple case as a set of points called landmarks. Depending on the definition of shapes, diverse shape spaces can be defined. Works as Kendall (1983): "Shape Manifolds, Procrustean Metrics, and complex Projective spaces" and Michor und Mumford (2004): "Riemannian geometries on spaces of plane curves," considered the space of shapes as a manifold. The main advantage of this approach is that we can use the basic tools of Differential Geometry: Riemannian metrics, Tangent, and Co-Tangent spaces, among others.

Motivated by PDE-constrained shape optimization problems, we propose a connected Discrete Shape Manifold representing a point set in R^d supporting a mesh with specific connectivity. In this work, we will present the fundamental properties of this manifold such as its topology and tangent space, among others. Our primary goal is to apply this definition to shape optimization problems. In this context, we will present a complete Riemannian metric which will guarantee to preserve the connectivity of the mesh along with bounded aspect ratios. The proposed algorithm will deform shapes following the geodesics over this manifold. Therefore a specific energy preserving scheme needs to be utilized for the numerical solution of the geodesic equation. Finally, some numerical experiments in 2D will be presented.

Multimaterial topology optimization based on the topological derivative

Peter Gangl (*Technische Universität Graz, Austria*)

09:50

The majority of shape and topology optimization algorithms considers the optimization with respect to two different states (e.g. material and void). In many engineering applications, however, one is interested in finding an optimal material distribution consisting of three or more different materials.

We present a multi-material topology optimization algorithm which is based on topological derivatives. Here, the design, which consists of more than two materials, is represented in an implicit way by a vector-valued level set function. We show a sufficient optimality condition and an iterative algorithm which is based on this condition. The algorithm can be seen as an extension of [Amstutz and Andrae, *J. Comp. Phys.* 2006, 216(2)] to multiple materials.

Finally, we show numerical results obtained by applying the algorithm to the optimization of an electric motor where the task is to find the optimal distribution of ferromagnetic material, air and permanent magnets.

Topology optimization of electrical machines with stress constraints

Jonas Holley (*Corporate Research, Robert Bosch GmbH, Germany, Humboldt-Universität zu Berlin, Germany*)

10:10

Michael Hintermüller (*WIAS Berlin, Germany*)

This talk focuses on mathematical optimization methods for finding the optimal design of the rotor of an electrical machine. The utilized approach is an adjoint-based topology optimization method following the topological derivative concept. Topological derivatives provide the sensitivity of an objective functional with respect to the creation of an infinitesimal small hole. Two physical domains are considered in the optimization problem. First, the electromagnetic torque is addressed. The underlying physical model are the two-dimensional magnetostatic equations. Second, the mechanical stresses in the rotor are included as pointwise state constraints. This extension is novel and crucial, especially in the context of industrial applications, in order to prevent material failure at high rotational speeds. The structural mechanical model employed for calculating the stresses are the equations of linear elasticity.

Regularizing the pointwise state constraints leads to an approximation of the original optimization problem, where the stresses are considered in the objective. The topological derivative of the resulting stress-based functional provides, together with the topological derivative of the electromagnetic objective, the sensitivity for a descent algorithm. A level set method is used as a framework for the optimization scheme.

S19.02 | Optimization of differential equations

Date: February 19, 2019

16:30-18:30

Room: HS 30

Shape optimization for interface identification with nonlocal system models

Christian Vollmann (*Universität Trier, Germany*)

16:30

Volker Schulz (*Universität Trier, Germany*)

Shape optimization methods have been proven useful for identifying interfaces in models governed by partial differential equations. For instance, shape calculus can be exploited for identifying diffusion coefficients, where the diffusivity is structured by piecewise constant patches.

On the other hand, nonlocal diffusion models, which are governed by integral operators instead of differential operators, have attracted increased attention in recent years. This is due to the large variety of applications including, e.g., peridynamics, image processing, nonlocal heat conduction or anomalous diffusion.

In this talk we bring together these two fields by considering a shape optimization problem, which is constrained by a nonlocal system model. We derive the shape derivative for the underlying integral equation and confirm theoretical results by numerical experiments.

Numerical methods for optimal design in conductivity

Marko Vrdoljak (*University of Zagreb, Croatia*)

16:50

Petar Kunštek (*University of Zagreb, Croatia*)

We consider optimal design problems for stationary diffusion in the case of two isotropic phases, with several state equations. The optimality of an arrangement is measured by an integral functional depending on the distribution of materials and the state functions. By relaxing the problem via homogenization method, an application of classical methods of calculus of variations is enabled, leading to optimality conditions and various numerical methods. However, in some special problem classes classical solutions occur, so it is reasonable to compare these numerical methods to ones which are based on shape derivative analysis, both first and second order methods.

Shape optimization in phosphate production

Nicolas Dietrich (*TU Kaiserslautern, Germany*)

17:10

Phosphate as an industrial product is an essential ingredient in, e.g., agriculture and the food industry. The production process is very energy consuming and takes place in high temperature melting furnaces. The costs of the productions are largely governed by energy costs of the furnace and there is a high potential to save energy by increasing the energy efficiency of the furnace. Naturally, the shape of the furnace has a high influence on its efficiency. In order to describe the temperature distribution within a furnace mathematically, a widely used model in the industry is the Rosseland approximation. We use this model and discuss the problem in the context of shape optimization.

Shape optimization for high temperature processes

Thomas Marx (*TU Kaiserslautern, Germany*)

17:30

High Temperature Processes have a wide field of applications in industrial processes, e.g., optimal control in glass cooling or shape optimization for melting furnaces. In order to improve the model accuracy compared with the standard Rosseland approximation, we consider here the SP_1 approximation. This leads to a PDE-constrained shape optimization problem, where the shape of the domain is the control variable. The optimal shapes are finally compared to the results obtained by the Rosseland approximation.

S19.03 | Optimization of differential equations

Date: February 20, 2019

08:30-09:30

Room: HS 30

Approximation of the Riccati operator for closed loop parabolic control problems

Helmut Harbrecht (*University of Basel, Switzerland*)

08:30

Ilja Kalmykov (*University of Basel, Switzerland*)

We consider the sparse grid approximation of the Riccati operator Π arising from closed loop parabolic control problems. In particular, we concentrate on the linear quadratic regulator (LQR) problems, i.e. we are looking for an optimal control u in the linear state feedback form $u(t, \cdot) = \Pi x(t, \cdot)$, where $x(t, \cdot)$ is the solution of the controlled partial differential equation (PDE) for a time point t . Under sufficient regularity assumptions, the Riccati operator Π fulfills the algebraic Riccati equation (ARE)

$$A\Pi + \Pi A - \Pi B B^* \Pi + Q = 0,$$

where A , B and Q are linear operators associated to the LQR problem. Furthermore, for certain control problems, Π can be expressed in terms of an integral kernel p . In such cases, the weak form of the ARE leads to a nonlinear partial differential equation for the kernel p - the Riccati PDE. Based on the available sparse grid software SG++, we are able to implement algorithms to solve the Riccati PDE with linear complexity $O(N)$ in the case of Dirichlet boundary control. Here, N is the number of degrees of freedom for the sparse grid representation of the integral kernel p .

A hybrid finite-dimensional RHC for stabilization of nonautonomous parabolic equations

Behzad Azmi (*Austrian Academy of Sciences, Austria*)

08:50

Karl Kunisch (*Austrian Academy of Sciences, Austria, University of Graz, Austria*)

One efficient strategy for dealing with optimal control problems on an infinite time horizon is the receding horizon framework. In this approach, the solution of an infinite-horizon problem is approximated through the concatenation of a sequence of open-loop optimal controls on overlapping temporal intervals. This talk is concerned with the stabilization of a class of time-varying linear parabolic equations by Receding Horizon Control (RHC). Here the range of RHC is finite-dimensional and RHC enters as a time-dependent linear combination of the finite numbers of

internal actuators. We discuss the stability and suboptimality of RHC with respect to the different choices of the control costs. In particular, we consider the case where the squared l_1 -norm as the control cost is chosen. This leads to a nonsmooth infinite-horizon problem which allows a stabilizing control with a low number of active actuators over time. Numerical experiments are also shown.

On oblique projection based stabilizing feedback control for nonautonomous systems

Sergio S. Rodrigues (*RICAM, OeAW, Austria*)

09:10

Recent results are presented concerning the explicit feedback stabilizability of nonautonomous nonlinear systems. The results concern both parabolic and coupled parabolic-ode systems. An example of such coupled systems are the monodomain equations, which we find in electrophysiology, as a model describing electric excitation and the propagation of electric waves in nerve fibers and in heart tissue. The control is a linear combination of a finite number of internal actuators. For coupled systems, the control acts only on the parabolic component. Results of simulations are presented showing the stabilizing performance of the feedback control, for both parabolic and coupled parabolic-ode systems. Optimization problems related to this class of feedback controls shall be discussed.

S19.04 | Optimization of differential equations

Date: February 20, 2019

14:00-16:00

Room: HS 30

Sparse discretization of sparse control problems

Evelyn Herberg (*University of Hamburg, Germany*)

14:00

Michael Hinze (*University of Hamburg, Germany*)

Henrik Schumacher (*RWTH Aachen, Germany*)

We consider optimal control problems that inherit a sparsity structure, especially we look at problems governed by measure controls. Our goal is to achieve maximal sparsity on the discrete level. We use variational discretization of the control problems utilizing a Petrov-Galerkin approximation of the state which induces controls that are composed of Dirac measures. In the parabolic case this allows us to achieve sparsity on the discrete level in space and time. Numerical experiments show the differences of this approach to a full discretization approach.

Numerical approximation of optimal control problems for hyperbolic conservation laws

Paloma Schäfer Aguilar (*TU Darmstadt, Germany*)

14:20

Stefan Ulbrich (*TU Darmstadt, Germany*)

Many physical problems, for example models for traffic or inviscid fluid flows, are described by hyperbolic conservation laws. We study boundary control problems where the initial and the boundary data are given by piecewise C^1 -functions, where the smooth parts as well as the switching times between the smooth parts serve as controls. It was shown by Pfaff and Ulbrich that under weak assumptions tracking-type objective functionals are differentiable with respect to the initial and boundary control and that the reduced gradient can be represented by the reversible solution of a suitable adjoint equation. In this talk, we discuss the consistent numerical approximation of these optimal boundary control problems for scalar hyperbolic conservation

laws, where we consider conservative finite difference schemes with corresponding sensitivity and adjoint scheme. To analyze the convergence of the adjoint schemes, we propose a convenient characterization of reversible solutions for the adjoint equation in the case of boundary control, which is based on the work of Bouchut and James for the initial value problem and is suitable to show that the limit of discrete adjoints is in fact the correct reversible solution of the adjoint equation. Furthermore we introduce a duality relation, which gives a uniquely characterization of the sensitivity by the reversible solution of the adjoint equation.

A priori error estimates for fracture control problem

Masoumeh Mohammadi (*TU Darmstadt, Germany*)

14:40

Winnifried Wollner (*TU Darmstadt, Germany*)

A control problem for a linearized time-discrete fracture propagation process is considered. The discretization of the problem is done using a conforming finite element method. In contrast to many works on discretization of PDE constrained optimization problems, the particular setting has to cope with the fact that the linearized fracture equation is not necessarily coercive. A quasi-best approximation result will be shown in the case of an invertible, though not necessarily coercive, linearized fracture equation. Based on this a priori error estimates for the control, state, and adjoint variables will be derived.

Reduced basis methods – an application to variational discretization of parametrized elliptic optimal control problems

Ahmad Ahmad Ali (*University of Hamburg, Germany*)

15:00

Michael Hinze (*University of Hamburg, Germany*)

We consider a class of parameter-dependent optimal control problems of elliptic PDEs with constraints of general type on the control variable. Applying the concept of variational discretization, together with techniques from the reduced basis method, we construct a reduced basis surrogate model for the control problem. We establish estimators for the greedy sampling procedure which only involve the residuals of the state and the adjoint equation, but not of the gradient equation of the optimality system. The estimators are sharp up to a constant, i.e. they are equivalent to the approximation errors in control, state, and adjoint state. Numerical experiments show the performance of our approach.

Multigoal-oriented error control in optimization problems with nonlinear PDE constraints

Bernhard Endtmayer (*Austrian Academy of Sciences, Austria*)

15:20

Ulrich Langer (*Austrian Academy of Sciences, Austria*)

Ira Neitzel (*Universität Bonn, Germany*)

Thomas Wick (*Leibniz Universität Hannover, Germany*)

Winnifried Wollner (*Technische Universität Darmstadt*)

In this presentation, we consider an optimal control problem subject to a nonlinear PDE constraint. Here, this constraint is given by the p-Laplace equation. Our goal is to design a method for treating multiple goal functionals. To this end, we derive a posteriori error estimates using dual weighted residual (DWR) method. Specifically, all goal functionals are combined to one single functional using an appropriate weighted combination. From the error estimator local error indicators are extracted that are then used for local mesh refinement. We substantiate our algorithmic development with some numerical tests.

This work has been supported by the Austrian Science Fund (FWF) under the grant P 29181 ‘Goal-Oriented Error Control for Phase-Field Fracture Coupled to Multiphysics Problems’ in collaboration with the DFG-SPP 1962 ‘Non-smooth and Complementarity-Based Distributed Parameter Systems: Simulation and Hierarchical Optimization’.

Adaptive optimization of FSI problems with reduced order models

Johanna Katharina Biehl (TU Darmstadt, Germany)

15:40

Stefan Ulbrich (TU Darmstadt, Germany)

The simulation and optimal control of fluid structure interaction problems is of interest in many engineering applications, as for example in medicine, civil engineering or aerodynamics. In this talk we present an adjoint-based multilevel SQP method [1,2] for Fluid Structure Interaction problems. We focus on incompressible fluid flows (modeled with the Navier-Stokes equations) and hyperelastic solids (e.g., Saint Venant-Kirchhoff materials). For these problems, we introduce a discretization based on a monolithic finite element method in space and a Crank-Nicolson scheme in time. Since this results in a large, nonlinear system, we want to reduce the computational time. To this end, the introduced multilevel SQP controls the accuracy of state and adjoint equation by adaptive grid refinement using residual based space-time error estimators. To speed up the optimization further, we approximate the current state and adjoint discretizations by a reduced order model (ROM), which is based on proper orthogonal decomposition (POD). The resulting ROMs are used within the optimization method to compute steps. The resulting algorithm is applied to a Benchmark problem proposed by Turek and Hron [3].

Acknowledgement. This work is supported by the ‘Excellence Initiative’ of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

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[2] S. Bott, Adaptive SQP Method with Reduced Order Models for Optimal Control Problems with Constraints on the State Applied to the Navier-Stokes Equations, Technische Universität Darmstadt, 2016, Dissertation

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S19.05 | Optimization of differential equations

Date: February 20, 2019

16:30-18:30

Room: HS 30

Finite element error estimates in $L^2(\Omega)$ for regularized discrete approximations to the obstacle problem

Dominik Hafemeyer (Technische Universität München, Germany)

16:30

Christian Kahle (Technische Universität München, Germany)

Johannes Pfefferer (Technische Universität München, Germany)

We consider the standard obstacle problem in a convex and polyhedrally bounded domain Ω with forcing $f \in L^\infty(\Omega)$, i.e. the variational inequality:

Find $u \in \mathcal{K}_\Psi := \{v \in H_0^1(\Omega) \mid v \geq \Psi \text{ a.e. in } \Omega\}$ such that

$$(\nabla u, \nabla(v - u)) \geq (f, v - u) \quad \forall v \in \mathcal{K}_\Psi. \quad (1)$$

Here $\Psi \in W^{2,\infty}(\Omega)$ is the given obstacle. Under the reasonable assumption of inactivity close to the boundary $\partial\Omega$ we derive quasi optimal error estimates for a numerical approximation of (1) based on a regularisation approach. Namely we obtain second order convergence (up to logarithmic terms) with respect to the spatial discretization, which is assumed to be quasi-uniform. No discrete maximum principle is required.

A model problem for optimal control of a parabolic PDE fully coupled to ODEs

Sven-Joachim Kimmerle (*Bundeswehr University Munich, Germany*)

16:50

In many applications we encounter fully coupled systems involving a partial differential equation (PDE) and an ordinary differential equation (ODE). Here we focus on a special model problem, where a parabolic PDE is fully coupled to ODEs that prescribe a time evolution, e.g., given by Newton dynamics. The volume source term of the PDE as well as a source term of the ODEs may be controlled. The controls are subject to box constraints.

We derive first-order necessary optimality conditions that exploit the particular structure of the problem comparing two approaches: to treat ODEs as PDEs or to consider PDEs as ODEs. Moreover, we discuss fixed point strategies, first-optimize-then-discretize vs. first-discretize-then-optimize approaches, the availability of explicit solutions and the challenges arising for these type of coupled optimal control problems. We close with numerical simulations and an outlook on more complicated real-world applications and their relation to our model problem.

A priori error estimates for an optimal control problem governed by a variational inequality of the second kind

Christian Meyer (*Technische Universität Dortmund, Germany*)

17:10

Monika Weymuth (*Universität der Bundeswehr München, Germany*)

We consider an optimal control problem governed by an elliptic variational inequality of the second kind. Based on differentiability properties of the solution map we derive strong stationarity conditions under quite mild assumptions on the active set. The optimal control problem is discretized by linear finite elements for the state and a variational discrete approach for the control. Finally we present a priori error estimates for the finite element discretization based on the strong stationarity conditions and a quadratic growth condition. The theoretical results are illustrated by numerical experiments.

Numerical analysis for parabolic time-optimal control problems with bang-bang controls

Boris Vexler (*Technical University of Munich, Germany*)

17:30

Lucas Bonifacius (*Technical University of Munich, Germany*)

Konstantin Pieper (*Technical University of Munich, Germany*)

In this talk we consider time-optimal control problems governed by parabolic partial differential equations. We concentrate on the formulation without a Tikhonov regularization term, which often leads to a bang-bang structure of the optimal control. We discretize the problem using a discontinuous Galerkin scheme in time and finite elements in space and provide a priori error estimates for this type of discretization. We illustrate our results with numerical examples.

S19.06 | Optimization of differential equations

Date: February 21, 2019

08:30-10:30

Room: HS 30

Optimal control of a rate-independent system constrained to balanced viscosity solutions

Stephanie Thomas (*University of Kassel, Germany*)

08:30

Dorothee Knees (*University of Kassel, Germany*)

We analyze an optimal control problem which is constrained to balanced viscosity (BV) solutions of a rate-independent system. This system is given in terms of a state variable $z: [0, T] \rightarrow Z$, a time-dependent external load l , a stored energy functional E depending on l and z , and a dissipation potential $R: Z \rightarrow [0, \infty)$, which captures the dissipation due to internal friction. The evolution of z can now be described by a doubly nonlinear differential inclusion involving the Gâteaux derivative of E with respect to z , and the convex subdifferential of R .

In rate-independent applications (e.g., dry friction, plasticity, fracture), the dissipative force does not depend on the velocity of the process, giving rise to a positively 1-homogeneous dissipation potential. We are further dealing with a semi-linear, but non-convex stored energy functional. In this case, we cannot expect continuous global energetic solutions, even if the external load is smooth. Therefore, we instead consider so-called BV solutions, which can be obtained via an approximation with viscously regularized systems.

We then show existence of solutions of an optimal control problem which is governed by the rate-independent system, where the external load serves as control variable. Since we constrain the problem to BV solutions, the focus is on the proof of compactness of the corresponding solution sets. In order to obtain the necessary a priori estimates, we introduce a reparametrization in such a way that the transformed solutions satisfy an autonomous rate-independent system on the non-negative real half line. We then obtain the essential estimates for solutions of this autonomous system by ODE-arguments and transfer them back to BV solutions.

Solving quadratic multi-leader-follower games by smoothing the follower's best response

Anna Thünen (*RWTH Aachen, Germany*)

08:50

Sonja Steffensen (*RWTH Aachen, Germany*)

Michael Herty (*RWTH Aachen, Germany*)

The multi-leader-follower game is a particular subset of classical game theory. These models serve as an analytical tool to study the strategic behavior of individuals in a noncooperative manner. In particular, the individuals (players) are divided into two groups, namely the leaders and the followers, according to their position in the game. Mathematically, this leads to optimization problems with optimization problems as constraints.

We derive Nash-s-stationary equilibria for a class of quadratic multi-leader-follower games using nonsmooth best response function. To overcome the challenge of nonsmoothness, we pursue a smoothing approach resulting in a reformulation as smooth Nash equilibrium problem. We prove existence and uniqueness for all smoothing parameter. For a decreasing sequence of this smoothing parameters accumulation points of Nash equilibria exists and we show that they fulfill the conditions of s-stationarity. Finally, we propose an update on the leader variables for efficient computation and numerically compare nonsmooth Newton and subgradient methods.

Optimal control of an abstract evolution variational inequality with application in homogenized plasticity

Christian Meyer (*Technische Universität Dortmund, Germany*)

09:10

Stephan Walther (*Technische Universität Dortmund, Germany*)

This talk is concerned with an optimal control problem constrained by an evolution variational inequality. The equations of plasticity and homogenized plasticity can be reduced to such an evolution variational inequality. Moreover, the flow rule is generalized by a maximal monotone operator. In particular, since the optimization problem is non-smooth, we consider a smoothed version of the problem in order to derive optimality conditions. To be more precise, we utilize the Moreau-Yosida regularization and show that solutions of the smoothed problem converge towards solutions of the original problem in a certain sense. For the smoothed problems, necessary first order optimality conditions involving an adjoint equation and sufficient second order optimality conditions will be presented.

On a PDE-constrained generalized Nash equilibrium problem with various multipliers

Veronika Karl (*Julius-Maximilians-Universität Würzburg, Germany*)

09:30

We apply an augmented Lagrange method to solve a PDE-constrained generalized Nash equilibrium problem. Under a Slater-type constraint qualification we prove an existence result. Further, we prove convergence of the applied method. We transfer and sharpen our results for the more special class of jointly convex GNEPs. Finally, the results are illustrated through numerical examples.

Exploitation of nonsmoothness in PDE-constrained problems instead of regularization

Olga Ebel (*Paderborn University, Germany*)

09:50

Andrea Walther (*Paderborn University, Germany*)

Stephan Schmidt (*Universität Würzburg, Germany*)

We consider nonsmooth PDE-constrained problems, where all non-differentiabilities are assumed to be caused by the nonsmooth operators $\text{abs}()$, $\text{min}()$ and $\text{max}()$.

Because of the sophisticated nature of such nonsmooth optimization problems very often substitute assumptions and regularization techniques are applied to avoid facing the intrinsic nonsmoothness.

The method under consideration is capable of solving this type of nonsmooth optimization problems without any regularization and additionally maintains reasonable convergence results.

The key idea is locating minimal solutions via an appropriate decomposition such that the so-called branch problems can be solved by standard optimization approaches, and additionally using the respective dual variables to update the switch between branch problems providing the minimal solution.

A bilevel approach for parameter learning in inverse problems

Gernot Holler (*University of Graz, Austria*)

10:10

Karl Kunisch (*University of Graz, Austria, Radon Institute, Austrian Academy of Sciences, Linz*)

Richard C. Barnard (*Western Washington University, Washington*)

We address a learning approach for choosing regularization weights in multi-penalty Tikhonov regularization of ill-posed inverse problems [1]. As motivating examples, we consider the inverse problems of estimating parameters in elliptic partial differential equations. Assuming that some ground truth data is given, the basic idea is to learn regularization weights by solving a bilevel (optimization) problem. Thereby, the lower level problem, which is depending on the regularization weights, is the Tikhonov regularized problem. In the upper level problem the distance of the lower level problem solutions to the ground truth data is minimized with respect to the regularization weights. In numerical experiments it was observed that regularization weights obtained by this procedure generalize well to structurally related data.

While bilevel problems are typically non convex, it is often assumed that at least the lower level problems are convex. However, this is in general not the case in the context of non linear parameter estimation problems. This leads to significant issues when deriving optimality conditions for the bilevel problem. We discuss these issues and describe how they can be resolved for specific examples. Results from numerical experiments are also presented. Finally, a brief outlook on related current work on learning nonlocal regularization operators is given, which is motivated by regularization with fractional order Sobolev semi norms.

References

[1] Gernot Holler, Karl Kunisch, and Richard C Barnard. A bilevel approach for parameter learning in inverse problems. *Inverse Problems*, 34(11):115012, 2018.

S19.07 | Optimization of differential equations

Date: February 21, 2019

14:00-16:00

Room: HS 30

Optimal medication for tumors modeled by a Cahn-Hilliard-Brinkmann equation

Patrik Knopf (*Universität Regensburg, Germany*)

14:00

Matthias Ebenbeck (*Universität Regensburg, Germany*)

We study a distributed optimal control problem for a diffuse interface model for tumor growth which was firstly proposed by M. Ebenbeck and H. Garcke. The model consists of a Cahn-Hilliard type equation for the phase field variable coupled to a reaction diffusion equation for the nutrient and a Brinkman type equation for the velocity. The system is equipped with homogeneous Neumann boundary conditions for the tumor variable and the chemical potential, Robin boundary conditions for the nutrient and a "No-friction" boundary condition for the velocity. The control acts as a medication by cytotoxic drugs and enters the phase field equation. The cost functional is of standard tracking type and is designed to track the variables of the state equation during the evolution and the distribution of tumor cells at some fixed final time. We prove that the model satisfies the basics for calculus of variations and we establish a first-order necessary optimality condition for the optimal control problem.

Assimilation of surface current and water level measurements into a 3d barotropic circulation model of the German Bight using a 4DVAR technique

Johannes Schulz-Stellenfleth (*Helmholtz-Zentrum Geesthacht (HZG), Germany*)

14:20

Because of the shallow water, the tidal dominated circulation in the German Bight is a challenge for numerical models. There are a lot of uncertainties about the bathymetry, as well as the bottom roughness, and the dynamics is complicated by strong nonlinear mechanism, like the

generation of overtides. At the same time, the German Bight is a very busy region with a lot shipping and offshore activities resulting in strong demands for accurate information on currents and water levels, i.e., in the context of Search and Rescue (SAR) operations.

In this study a combination of tide gauge observations and measurements from three HF radar stations in the German Bight are assimilated into a 3D circulation model with 1 km resolution and 7 vertical layers in order to improve estimates for water levels and currents. The horizontal grid and bathymetry as well as the open boundary and meteo forcing is identical to the setup used at the Hydrographic Federal Maritime and Hydrographic Agency (BSH). A 4DVAR technique is used, which is based on an adjoint model to compute the gradient of a cost function, which penalizes deviations between the observations and the model results.

The analysis is performed in two steps, where systematic model errors like bottom roughness, internal friction related to turbulence and meteo drag coefficients are treated first. For this purpose, the system is run in a hindcast mode over a certain tuning period. Subsequently, stochastic error components relevant in an operational forecast setup, like errors in the open boundary forcing and the meteo forcing are reduced. This is done in a forecast configuration where a 12 hour forecast is launched based on a 12 hour hindcast.

The results are compared to the operational output of the BSH system as well as to drifter data acquired in 2015. The achieved improvements, as well as remaining residuals between model and observations are discussed. Particular focus is put on the spatial distribution of remaining systematic errors and strategies to further reduce these.

Arbitrary sensitivity for inverse problems in piezoelectricity

Benjamin Jurgelucks (*Paderborn University, Germany*)

14:40

Veronika Schulze (*Paderborn University, Germany*)

Nadine Feldmann (*Paderborn University, Germany*)

Leander Claes (*Paderborn University, Germany*)

For the development of new piezoelectric ceramics accurate knowledge of its material parameters are indispensable. However, current material parameter identification methods which are based on the solution of inverse problems commonly cannot retrieve all material parameters. One reason for this behavior is that some material parameters have a very low or zero sensitivity with respect to the measurable quantity of the inverse problem.

In order to overcome this issue a triple-ring electrode setup for disk-shaped piezoceramics was suggested which increases the sensitivity with respect to all parameters. However, the sensitivity now depends on the exact electrode geometry of the three rings which can be increased in an optimization problem.

Moreover, a novel method is presented which guarantees arbitrary sensitivities based on the previously optimized electrode geometry.

Numerical identification of motor units in muscles

Tobias Sproll (*University Bayreuth, Germany*)

15:00

Anton Schiela (*University Bayreuth, Germany*)

Madeleine Lowery (*University College Dublin, Ireland*)

High density surface Electromyography (sEMG), is a non-invasive method of measuring the activity of muscles whereby an array of electrodes is placed above the skin and a spatially and temporally resolved measurement of the electric potential on the skin is obtained. Recent advances in high-density sEMG measurement have opened the possibility of extracting information about single motor units (groups of muscle fibers controlled by the same motor neuron) from the sEMG signal.

In this talk we present a mathematical approach to identify these motor units from measurements. On base of an electrostatic forward model we discuss an optimal control approach. For this optimal control problem we will discuss the existence of a solution in the case of an H^2 -regular control.

Controlling a crowd with stochastic influence using external agents

Claudia Totzeck (*TU Kaiserslautern, Germany*)

15:20

We discuss a control algorithm based on space-mapping to guide a crowd that undergoes stochastic influence with the help of external agents. The crowd is modelled by a large system of stochastic differential equations (SDE) which are coupled to ordinary differential equations (ODE) representing the external agents. The control variables are the velocities of the external agents. Due to the stochastic nature of the model, it is not possible to use a straight forward extension of approaches developed for the Optimal Control with ODE as constraints. Our work-around is based on the space-mapping approach which will be discussed in detail. Promising numerical results justify the proposed method.

Optimization problems for interacting particle systems and corresponding mean-field limits

René Pinnau (*TU Kaiserslautern, Germany*)

15:40

We investigate optimal control problems constrained by a system of ODEs modelling interacting particles. In particular, we are interested in the limiting mean-field optimal control problem as the number of particles tends to infinity. Special focus is on the derivation of the corresponding first-order optimality systems in different functional analytical settings. Several links between the different approaches are shown and their numerical applicability is discussed.

S19.08 | Optimization of differential equations

Date: February 22, 2019

08:30-10:30

Room: HS 30

Optimal control and asymptotic analysis of the Cattaneo model

Sebastian Blauth (*Fraunhofer ITWM, Germany*)

08:30

In this talk we investigate an optimal control problem for the Cattaneo equation, which is used in order to model delayed heat transfer. Our main topic is the asymptotic analysis of an optimal control problem for a vanishing delay time. In particular, the convergence of both optimal states and controls for the Cattaneo equation to the ones for the heat equation is shown. Furthermore, we also take a look at the numerical solution of the optimal control problem for the Cattaneo equation, again focusing on the asymptotic behavior of the solutions.

The Cattaneo-Model in the context of thermoablation of liver tumors

Matthias Andres (*Technische Universität Kaiserslautern, Germany*)

08:50

René Pinnau (*Technische Universität Kaiserslautern, Germany*)

Laser-induced thermotherapy is a medical treatment which attempts to destroy liver tumors by thermal ablation. The heat transfer inside the liver is classically described by a nonlinear coupling of the so-called bio-heat equation and a radiative transfer model. In order to control the speed of heat propagation we consider an additional term for the second-order time derivative of the solution and obtain a Cattaneo-like model. For this we investigate the problem of parameter identification in terms of PDE-constrained optimization.

Optimal boundary control of hyperbolic balance laws with state constraints

Johann Michael Schmitt (*TU Darmstadt, Germany*)

09:10

Stefan Ulbrich (*TU Darmstadt, Germany*)

This talk deals with the treatment of pointwise state constraints in the context of optimal boundary control of nonlinear hyperbolic scalar balance laws. We study an optimal control problem governed by balance laws with initial and boundary conditions, where we suppose that the boundary data switch between smooth functions at certain switching points. The smooth functions and the switching points are hereby considered as the control. The appearance of state constraints presents a special challenge, since solutions of nonlinear hyperbolic balance laws may develop discontinuities after finite time, which prohibits the use of standard methods. In this talk, we will build upon the recently developed sensitivity- and adjoint calculus by Pfaff and Ulbrich to derive necessary optimality conditions. In addition, we will use Moreau-Yosida regularization for the algorithmic treatment of the pointwise state constraints. Hereby, we will prove convergence of the optimal controls and weak convergence of the corresponding Lagrange multiplier estimates of the regularized problems.

Optimal control of a critical semilinear wave equation in 3d

Hannes Meinlschmidt (*RICAM Linz, Austria*)

09:30

Karl Kunisch (*RICAM Linz, Austria, Karl-Franzens-Universität Graz, Austria*)

We consider optimal control problems subject to a defocusing H^1 critical semilinear wave equation on a domain in three spatial dimensions. The prototype nonlinearity here is of power type with exponent 5. The control enters linearly and we have homogeneous Dirichlet- or Neumann boundary data. A natural control space would be L^1 in time and L^2 in space. The critical exponent 5 makes global analysis for the equation under consideration difficult, and global existence for $u = 0$ has been shown only recently. We discuss the solution concept for the PDE and optimality conditions.

Optimal control of the relativistic Vlasov-Maxwell system with boundary conditions

Jörg Weber (*University of Bayreuth, Germany*)

09:50

The time evolution of a collisionless plasma is modeled by the relativistic Vlasov-Maxwell system, which couples the Vlasov equation (the transport equation) with the Maxwell equations of electrodynamics. The plasma particles are located in a bounded domain, for example a fusion reactor. In the exterior, there are external currents that may serve as a control of the plasma if adjusted suitably. Also, we allow material parameters, that is to say permittivity and permeability, which may depend on the space coordinate. We discuss solution theory of the modeling nonlinear PDE system. Unfortunately, there is only a very weak solution concept and uniqueness of solutions to the initial value problem is not known. This causes many problems when treating an optimal control problem, on which the main focus of this talk lies. On the one hand, particles hitting the boundary of their container and thus causing damage, and, on the other hand, exhaustive control costs are penalized. We prove existence of minimizers of the arising minimizing problem and give an approach to derive first order optimality conditions.

S20 | Dynamics and control

Organiser: Sergio Lucia (*Technische Universität Berlin, Germany*)
Roman Geiselhart (*Ulm University, Germany*)

S20.01 | Dynamics and control

Date: February 19, 2019
Room: HS 05

08:30-10:30

H2-optimal model order reduction of interconnected systems

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*) 08:30
Sara Grundel (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Petar Mlinarić (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

We consider interconnected systems, network systems of linear time-invariant subsystems, coupled linearly through their inputs and outputs. For linear time-invariant systems, the two-sided iteration algorithm is a locally H2-optimal model order reduction method. It is based on the Wilson conditions, which are necessary H2-optimality conditions in the form of matrix equations. We derive Wilson-type necessary optimality conditions for H2-optimal structure-preserving model order reduction of interconnected systems. Furthermore, we discuss solution methods, in particular the gradient descent method.

Model reduction of district heating using network decomposition

Markus Rein (*TU Kaiserslautern, Germany, Fraunhofer Institute for Industrial Mathematics ITWM, Germany*) 08:50
Jan Mohring (*Fraunhofer Institute for Industrial Mathematics ITWM, Germany*)
Tobias Damm (*TU Kaiserslautern, Germany*)
Axel Klar (*TU Kaiserslautern, Germany*)

In this contribution we study the model order reduction of nonlinear transport networks at the example of district heating. In these, energy injected at a centralized power plant is transported to consumers, building a hyperbolic differential algebraic system with large state space dimension. The network structure introduces sparse system dynamics, which transform to a dense reduced system leading to unfeasible computational costs [1]. To exploit the benefits of sparsity, sub-parts of the network are reduced separately in a structure preserving way using Galerkin projection [2]. Concerning the network partitioning [3], we analyze strategies that are suitable for the transport character of the dynamics. The resulting reduced order model is an efficient surrogate for the optimal control of district heating networks.

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Filtering and model order reduction of PDAEs with stochastic boundary data

Nadine Stahl (*Trier University, Germany*)

09:10

Nicole Marheineke (*Trier University, Germany*)

State reconstruction using model hierarchies is an open field of research, which we address in this talk. Proceeding from models of partial differential equations with stochastic boundary data (e.g. gas networks), spatial discretization yields differential-algebraic descriptor systems driven by a white noise valued input. By help of model order reduction techniques, model hierarchies can be established. In view of model-predictive control, we investigate the performance of state reconstruction based on this hierarchy. Of special interest hereby are the relationship between the quality of the state estimation and the underlying reduced order model as well as the influence of the algebraic constraints.

Semi-active H_∞ damping optimization by adaptive interpolation

Zoran Tomljanović (*University of Osijek, Osijek, Croatia*)

09:30

Matthias Voigt (*Technische Universität Berlin, Germany*)

We consider the problem of semi-active damping optimization of mechanical systems. The main problem is to determine the best damping matrix which will minimize the influence of the input to the output of the system. We use a minimization criteria based on the H_∞ system norm. Since that the objective function is a non-convex function, this damping optimization problem usually requires a large number evaluations of objective function. Thus, we will be focused on fixed damper positions and we will investigate efficient optimization of damping viscosities. Our main goal is to compute a damping that is locally optimal with respect to the H_∞ -norm of the transfer function from the exogenous noise inputs to the performance outputs. We make use of a new greedy method for computing the H_∞ -norm of a transfer function based on rational interpolation. Our approach is particularly adapted to parameter-dependent transfer functions. The interpolation leads to parametric reduced-order models that can be more efficiently optimized. At the optimizers we then take new interpolation points to refine the reduced-order model and to obtain updated optimizers. We also consider different heuristics for choosing initial interpolation points. In our numerical examples we show that this approach normally converges fast and thus can highly accelerate the optimization procedure.

Fixed order H-infinity controller design for delay systems

Paul Schwerdtner (*TU Berlin, Germany*)

09:50

Matthias Voigt (*TU Berlin, Germany*)

In this talk, we present an algorithm that is used to compute fixed order controllers for delay systems that minimize the H-infinity norm of the closed loop transfer function. Specifically, we alter the controller parameters of a given fixed order controller with possibly structural constraints to optimize the H-infinity-performance of the resulting closed loop transfer function using direct numerical optimization. For that, we use a recently developed algorithm for the computation of H-infinity-norms of irrational functions such as transfer functions of systems with delay. It is based on rational interpolation using the Loewner matrix framework. After a brief explanation of the H-infinity computation method, we show how its properties can be used efficiently in an optimization loop for the synthesis of robust controllers of delay systems, outperforming the currently available algorithm for this purpose. After that, the applicability of the developed method for a broader class of systems is presented and the realization independence of the

utilized algorithm for the H-infinity-norm computation is exploited to also impose performance requirements on transfer functions of closed loop systems using weight functions in the delay setting.

Polynomial approximation of Isaacs' equation and applications to control under uncertainty

Dante Kalise (*Imperial College London, United Kingdom*)

10:10

Sudeep Kundu (*University of Graz, Austria*)

Karl Kunisch (*University of Graz, Austria, Johann Radon Institute for Computational and Applied Mathematics, Linz, Austria*)

We propose a numerical scheme for the approximation of high-dimensional, nonlinear Isaacs PDEs arising in robust optimal feedback control of nonlinear dynamics. The numerical method consists of a global polynomial ansatz together separability assumptions for the calculation of high-dimensional integrals. The resulting Galerkin residual equation is solved by means of an alternating Newton-type/policy iteration method for differential games. We present numerical experiments illustrating the applicability of our approach in robust optimal control of nonlinear parabolic PDEs.

S20.02 | Dynamics and control

Date: February 19, 2019

16:30-18:30

Room: HS 05

CANFIS based semi-active vibration control of stochastically excited high-rise civil engineering structures with nonlinearities and uncertainties

Okyay Altay (*RWTH Aachen University, Germany*)

16:30

Sven Klinkel (*RWTH Aachen University, Germany*)

This paper presents an optimal feedback vibration control strategy for high-rise civil engineering structures, such as buildings, wind turbines and towers. The proposed system uses semi-active dampers, which are distributed in the structure. Due to their adaptation capability, semi-active dampers perform more efficiently than passive and active dampers; however, their parameter adaptation requires sophisticated control strategies.

The main reason for this requirement is the highly nonlinear behavior of semi-active dampers. Additionally, mathematical models of these dampers involve significant uncertainties especially regarding the inherent damping processes. Moreover, the response of high-rise structures to strong excitations, such as earthquake, high winds and explosion, can also be nonlinear due to the plastic deformations of the structural components.

Previous studies have shown that fuzzy logic controllers (FLC) can overcome these challenges and perform effectively with semi-active dampers to mitigate the structural vibrations involving nonlinearities and uncertainties. Nevertheless, FLC require a predefined tuning of their fuzzy rules and membership functions, which must be performed based on the knowledge of a human expert. Combining FLC with artificial neural networks (ANN), adaptive neuro-fuzzy systems are proposed, which can determine autonomously and efficiently the parameters of FLC by using learning based training and adaptation strategies of ANN. However, there is only limited research investigating the performance of these adaptive systems in the field of vibration control of civil engineering structures.

The present work is concerned with a numerical formulation of such an adaptive system, in particular a co-active neuro-fuzzy inference system (CANFIS), and its implementation on a non-linear seismically excited three-story steel benchmark building. As a multiple input multiple

output (MIMO) system, the accelerations of each story used as feedback signals for the controller inputs. To reduce the horizontal vibrations of the building, three vertically distributed independent semi-active dampers are used, which can adapt their damping forces according to the control signals. The performed simulations consider the delays, which occur both in the measured signals and during the generation of the control forces. Error backpropagation is applied as a learning method to train beforehand the premise and consequent parameters of the controller while minimizing a quadratic cost function. The performance of the proposed control system is subsequently verified by analyzing the response time-histories of the benchmark structure to representative historical earthquake records. In this study, with the proposed hybrid vibration control policy a significant reduction of the peak roof displacements of 81.7 % to 89.1 % is achieved.

Control of structural displacements by eigenstrains in the presence of propagating singular waves: uni-axial motion

Hans Irschik (*Johannes Kepler Universität Linz, Austria*)

16:50

Andreas Brandl (*Johannes Kepler Universität Linz, Austria*)

The present paper deals with the control of structures by eigenstrains. We restrict to a feed-forward scenario, in which imposed loadings as well as the structural parameters can be considered as known. We wish to demonstrate that and how displacements can be controlled, when propagating singular waves would be present in the uncontrolled case. To our best knowledge, this is a novel topic; in our present preliminary study, we restrict to the uni-axial case of wave propagation in straight linear elastic rods, see e.g. Bedford and Drumheller[1] for basic relations in the absence of eigenstrains. The latter can be inferred by analogy to thermal loadings, see e.g. Parkus [2], who also discussed the relations of jump that must hold at a propagating singular wave front. In practice, control by eigenstrains appears to be most promising in connection with smart structures technology, e.g. considering a piezoelectric actuation instead of a thermal one. Not discussing technological issues, our present contribution however remains in the theoretical framework of uni-axial linear elasticity in the presence of eigenstrains, the solution of our problem being a necessary prerequisite for possible future applications in practice. Utilizing symbolic computations, we first present cases, for which shock and acceleration wave fronts do propagate in rods. From these examples, it is seen that such singular waves, when produced by force loadings, can be indeed annihilated by proper eigenstrain actuations. Considering uniqueness requirements for the linear problems at hand, we derive necessary and sufficient conditions for the eigenstrains, in order that the displacements are controlled also when shock and acceleration wave fronts would result from imposed force loadings in the uncontrolled case. It turns out that the eigenstrains, written in the form of actuation stresses, must satisfy certain quasi-static equilibrium conditions, together with certain relations of jump at the propagating wave fronts. This result extends previous findings of our group concerning the control of displacements by eigenstrains in the absence of propagating singular wave fronts, see [3] and [4].

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External vibration damping of a robot manipulator's TCP using acceleration feedback

Tobias Franz Christian Berninger (*Technical University of Munich, Germany*)

17:10

Daniel Jean Rixen (*Technical University of Munich, Germany*)

There are multiple possible applications, which demand high accuracy from industrial robot arms. The usual approach to improve the path accuracy of these robot manipulators is to make the mechanical design as stiff as possible and to employ high fidelity joint controllers, which compensate path inaccuracies with well-identified models of the manipulator system. These methods are, however, only available to the robot manufactures themselves during their development phase. Companies designing tools for specific high accuracy tasks generally cannot change the design of a given robot manipulator and are bound to its precision. An alternative concept to further increase the path accuracy of a robot manipulator, without making changes to its design itself, might be to employ traditional Active Vibration Damping techniques by adding a supplementary proof-mass actuator to the robots tool center point with collocated acceleration sensor feedback.

This contribution explores the feasibility of this idea within a multi body simulation of a simple robot manipulator, which consist of rigid links, flexible joints and is actuated by cascaded joint controllers. The performance of an acceleration feedback controller employed on the robots TCP is evaluated by a test trajectory. The influence of the varying system dynamics during pose change of the robot are investigated, as well as the possible interaction between the joint controllers and the external active vibration controller.

Mixed control of vibrational systems

Ivica Nakić (*University of Zagreb, Croatia*)

17:30

Ninoslav Truhar (*University of Osijek, Croatia*)

Zoran Tomljanović (*University of Osijek, Croatia*)

We consider new performance measures for vibrational systems based on the H_2 norm of linear time invariant systems. New performance measures will be used as an optimization criterion for the optimal damping of vibrational systems. We consider both theoretical and concrete cases in order to show how new performance measures stack up against the standard measures. The quality and advantages of new performance measures as well as the behaviour of optimal damping positions and corresponding damping viscosities are illustrated in numerical experiments.

Model-free adaptive control method applied to vibration reduction of a flexible crane as MIMO system

Hoang Anh Pham (*University of Duisburg-Essen, Germany*)

17:50

Dirk Söffker (*University of Duisburg-Essen, Germany*)

Model-free adaptive control (MFAC) approaches are able to be used when system models are not available. This avoids to require exact mathematical models with respect to consideration of modeling errors even in the case of nonlinear systems to be controlled. The control strategy denoted as model-free when for controller design only the available system data is used. In this contribution, based on the knowledge of MFAC, an extension of the existing approach will be presented and applied to unknown multivariable system. The main idea of this method is that estimation of a time-varying parameter which represents the system dynamics by using only the

system inputs and outputs. Then, a novel control input algorithm is computed by minimizing both of the output tracking errors and its variations. The designed controller is applied to a flexible crane, representing a class of MIMO systems. The simulation results demonstrate that the vibrations of a crane system could be reduced significantly.

S20.03 | Dynamics and control

Date: February 20, 2019
Room: HS 05

08:30-09:30

Funnel control for linear non-minimum phase systems

Thomas Berger (*Universität Hamburg, Germany*)

08:30

We consider tracking control for linear systems with known relative degree which are possibly non-minimum phase, i.e., their zero dynamics may have an unstable part. For a given sufficiently smooth reference signal we design a low-complexity controller which achieves that the tracking error evolves within a prescribed performance funnel. We present a novel approach where a new output is constructed, with respect to which the system has a higher relative degree, but the unstable part of the internal dynamics is eliminated. Using recent results in funnel control, we then design a controller for this new output, which also incorporates a new reference signal. We prove that the original output stays within a prescribed performance funnel around the original reference trajectory and all signals in the closed-loop system are bounded. The results are illustrated by some simulations.

Funnel control for boundary observation and control systems

Marc Puche (*University of Hamburg, Germany*)

08:50

The funnel controller is a well-known adaptive controller which tracks a prescribed reference signal, so that the error between the output and the signal remains enclosed within a funnel boundary. So far it has been proved to be applicable for a large class of finite dimensional, nonlinear systems. Here, we present recent results about the feasibility of the funnel controller for a wide class of systems whose state is described by a partial differential equation (PDE) and the observation and control occur at the boundary. Moreover, the fact of considering this general setting of boundary control and observation systems (BCOS) enables us to deal with both hyperbolic and parabolic PDEs in a unified framework. The mathematical tools used to prove the main result are based on the theory of nonlinear m -dissipative operators in Hilbert spaces. We conclude by showing simulations of three different systems.

Asymptotic tracking with funnel control

Stephan Trenn (*University of Groningen, Netherlands*)

09:10

Funnel control is a strikingly simple control technique to ensure model free practical tracking for quite general nonlinear systems. It has its origin in the adaptive control theory, in particular, it is based on the principle of high gain feedback control. The key idea of funnel control is to chose the feedback gain large when the tracking error approaching the prespecified error tolerance (the funnel boundary). In fact, the feedback gain goes to infinity when the distance between the error signal and the funnel boundary approaches zero. As a consequence, by letting the funnel boundary tending to zero asymptotically (to achieve asymptotic tracking), the feedback gain grows unbounded because the distance between error and funnel boundary necessarily converges

to zero. It was long believed that this is a theoretical limitation of funnel control, however, in this contribution it will be shown that this is not the case: It is possible to achieve asymptotic tracking with funnel control (i.e. without using the internal model principle) while all involved control signals remain bounded.

S20.04 | Dynamics and control

Date: February 20, 2019

14:00-16:00

Room: HS 05

Foundations and applications of infinite-dimensional input-to-state stability theory

Andrii Mironchenko (*Universität Passau, Germany*)

14:00

During the last three years, the input-to-state stability (ISS) theory of infinite-dimensional systems has been developing at a staggering pace.

Fundamental theoretical tools have been developed on the basis of semigroup and admissibility theories, Lyapunov methods, and PDE theory. These tools allow us to investigate robust stability and stabilization of linear and nonlinear PDEs of parabolic and hyperbolic type, ODE-PDE and PDE-PDE cascades as well as PDEs with moving boundaries, both with boundary and distributed disturbances. This makes ISS theory for distributed parameter systems an ideal basis for the study of heterogeneous interconnected systems with boundary and in-domain couplings. In this talk, we give an overview of the state of the art of the infinite-dimensional ISS theory and describe challenging open problems within this field.

An ISS characterization for discontinuous discrete-time systems

Roman Geiselhart (*Ulm University, Germany*)

14:40

Navid Noroozi (*Otto-von-Guericke University Magdeburg, Germany*)

Input-to-state stability (ISS) is an important concept to study robustness properties of nonlinear control systems. Among other things, the reason for its importance is the existence of an equivalent characterization in terms of ISS Lyapunov functions. For discrete-time nonlinear control systems two different forms of ISS Lyapunov functions (implication-form and dissipation-form) are known to be equivalent if the dynamics are continuous. However, for discontinuous dynamics the equivalence is no longer satisfied. In this work, we discuss this phenomenon and, eventually, give a complete characterization of ISS. Four different forms of ISS Lyapunov functions are presented and shown to be equivalent under a condition called global \mathcal{K} -boundedness. Most importantly, this condition is shown to be necessary for input-to-state stability.

Last but not least, we are interested in ISS with respect to closed sets. In that way, we recover several stability properties such as incremental stability, partial stability and independent-input-to-output stability in a unified manner.

Optimal control of nonlinear dissipative systems

Frédéric Enrico Haller (*Universität Hamburg, Germany*)

15:00

We revisit the nonlinear optimal control problem for time-variant nonlinear differential-algebraic systems on finite time-horizon. We follow the so-called system space approach, which already has been studied in the linear-quadratic case and we derive the corresponding Hamilton-Jacobi-Bellman equation. We also establish a link between this approach in the time-invariant case to the theory of dissipative systems. We illustrate the latter by applying the findings to time-invariant nonlinear RLC-circuits.

Tracking of non-feasible curves for underactuated nonlinear systems

Victoria Grushkovskaya (*Julius Maximilian University of Würzburg, Germany, National Academy of Sciences of Ukraine, Ukraine*)

15:20

Alexander Zuyev (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany, National Academy of Sciences of Ukraine, Ukraine*)

This talk focuses on the development of stability conditions for nonlinear non-autonomous systems of ordinary differential equations and their applications to control problems.

In the first part of the talk, we present a novel approach for the study of the asymptotic stability properties for nonlinear non-autonomous systems based on considering a parameterized family of sets [1,2]. In particular, we state local and global asymptotic stability conditions for a family of sets representing the level sets of a time-varying Lyapunov function. These results extend the stability conditions obtained in [1] for gradient-like systems to general nonlinear non-autonomous systems. We also study several special cases and provide asymptotic stability conditions in a neighbourhood of a given curve, which is in general not a trajectory of the system. The proposed approach allows to estimate the rate of convergence of solutions to a prescribed neighbourhood of the curve.

In the second part of the talk, we demonstrate the application of the obtained results to several control problems. In particular, we present a constructive solution to the trajectory tracking problem for a class of nonholonomic systems. Exploiting the control design strategy from [3] and the obtained stability conditions, the presented control approach allows to stabilize a system in a prescribed neighbourhood of a given curve, which not necessarily corresponds to a feasible trajectory of the system. Moreover, we also consider an extremum seeking problem, where the goal is to track the minimum of a time-varying cost function using gradient-free controllers [1].

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A smooth start method for spherical robot based on sliding mode control

Ting Zhou (*Beijing Jiaotong University, China*)

15:40

Yugong Xu (*Beijing Jiaotong University, China*)

Bin Wu (*Beijing Jiaotong University, China*)

This paper aimed at the problem that spherical robot moved in the opposite direction at the start-up stage proposed a new variable rate reaching law similar to the Gaussian function also a hierarchical sliding mode controller based on the new reaching law is given. Without increase adjust time of control system, the controller based on the new reaching law has a lower output when controlled state variable at start-up stage and near the desired value than one under conventional reaching laws, thus reduce the opposite direction displacement of spherical robot at the start-up stage and suppress chattering caused by the discontinuity of switch function. The comparisons among the new reaching law, constant rate reaching law and exponential reaching law and the effects of different parameters on the performance of new reaching law are given to reveal convergence characters of the new reaching law. The global stability of the closed-loop control system is proved by Lyapunov theory. To verify the method's effectiveness, the comparisons on controllers in different reaching law are presented, and the results demonstrate this new reaching law is valid.

S20.05 | Dynamics and control

Date: February 20, 2019

16:30-18:30

Room: HS 05

Approximation of output-feedback robust model predictive controllers via deep learning

Benjamin Karg (*TU Berlin, Germany*)

16:30

Sergio Lucia (*TU Berlin, Germany*)

Handling uncertainties is one of the most important challenges in nonlinear model predictive control (NMPC). While several methods have been recently presented, their implementation is usually difficult due to the necessary conservative assumptions or because of the required computational complexity.

In this work, we use a complex robust NMPC approach based on stochastic programming to generate data pairs that are used to learn and approximate a robust controller which is robust to model uncertainties and disturbances. We propose to use deep neural networks to learn the approximate controller motivated by recent results that prove the powerful representation capabilities of such networks over traditional shallow ones.

We suggest different alternatives to take into account the approximation errors to achieve solutions that can guarantee the satisfaction of the constraints. Finally, we show how an estimator can be designed independently or jointly with the approximated controller to achieve a high-performance predictive control of low complexity. The potential of the approach is illustrated with numerical results for the embedded robust control of different case-studies.

Specialized adaptive algorithms for the model predictive control of PDEs

Lars Grüne (*University of Bayreuth, Germany*)

16:50

Manuel Schaller (*University of Bayreuth, Germany*)

Anton Schiela (*University of Bayreuth, Germany*)

Model Predictive Control (MPC) is a control method in which the solution of optimal control problems on infinite or indefinitely long horizons is split up into the successive solution of optimal control problems on relatively short finite time horizons. Only a first part with given length of this solution is implemented as a control for the longer, possibly infinite horizon.

Motivated by this application, we want to construct adaptive algorithms for the solution of optimal control problems governed by parabolic partial differential equations which are tailored to this MPC-context. More specifically, as the feedback entering the system is the initial part of the control, we employ goal oriented error estimation to obtain high accuracy of this feedback while keeping the numerical effort low.

In this talk, we will present algorithms motivated by theoretical results and evaluate their performance in different numerical examples.

Vision- and MPC-based control of a power-cube serial robot

Jörg Fehr (*Universität Stuttgart, Germany*)

17:10

Patrick Schmid (*Universität Stuttgart, Germany*)

Georg Schneider (*Universität Stuttgart, Germany*)

Peter Eberhard (*Universität Stuttgart, Germany*)

Currently, the interaction between man and machine is a field of high topicality. Cage-free robots are developed to collaborate literally hand in hand with humans.

For a reasonable usage of robots, three aspects are important: modeling, sensing, and actuation. Modeling plays an important role in the development process as well as for controlling the robot, e.g., for model-based control concepts like model predictive control (MPC). This control technique uses the advantageous capability of the derived model to forecast the future dynamical behavior of the system and provides an optimal input based on solving an optimization problem during each sampling interval. In contrast to decentralized linear joint controllers, the advantages of a centralized MPC are given by simple handling of multivariable control problems, considering actuator limitations and systematic adjusting of controller parameters. Sensing is important for controlling the robot on the one hand, and for monitoring the environment on the other hand. Both can be realized by camera-based systems that detect positions of robots, humans, and workpieces, leading to safer and faster workflows.

In this contribution, both MPC and a vision based approach for gaining control feedback in real-time are combined for a serial manipulator in an experimental study. Deriving the predictive control law includes a structured step-by-step design procedure involving parameter identification and derivation of the forward and inverse dynamics. To handle the heavy online computational burden originating from the derived nonlinear model, a linear time-varying MPC scheme is developed based on linearizing the nonlinear system with respect to the desired trajectory and the a-priori known corresponding feed-forward controller. Instead of using the angles measured by the built-in incremental sensors of the robot as feedback for the MPC controller, the current pose of the robot is detected based on images from a low-cost industrial camera. For this purpose, the robot is equipped with three markers, which can be detected by means of color filtering during image processing. From the image coordinates of the detected markers, the joint angles are calculated and fed back to the controller.

The work shown in this contribution can be realized in a lean and cheap manner by standard hardware and is part of our overall research on safety-critical man-machine interaction.

Optimal control of differential-algebraic system using regularization techniques

Achim Ilchmann (*TU Ilmenau, Germany*)

17:30

Jonas Witschel (*TU Ilmenau, Germany*)

Karl Worthmann (*TU Ilmenau, Germany*)

We consider the linear-quadratic Optimal Control Problem (OCP) for systems governed by differential-algebraic equations. Using the feedback equivalence form or the regularization technique proposed by Berger and Van Dooren, we characterize the regularity of the generalized input and the space of consistent initial conditions to transform the OCP into an equivalent OCP solely constrained by ordinary differential equations, which can then be solved using classical results from linear quadratic control.

Model predictive control for linear differential-algebraic equations based on regularisation

Achim Ilchmann (*Technische Universität Ilmenau, Germany*)

17:50

Jonas Witschel (*Technische Universität Ilmenau, Germany*)

Karl Worthmann (*Technische Universität Ilmenau, Germany*)

We are concerned with Model Predictive Control (MPC) for systems governed by Differential-Algebraic Equations. Hereby, we employ a recently proposed regularisation technique to rewrite the optimal control problem to be solved in each MPC step into an equivalent one, in which the system dynamics are given by ordinary differential equations. Based on this new representation,

state and control constraints can be tackled by suitably constructing terminal constraints and costs such that asymptotic stability of the MPC closed loop is guaranteed. While doing so, the input and its regularity are identified and classified.

Cycle-based adaption of a model-predictive control strategy for injection molding machines

Christoph Froehlich (*TU Wien, Austria*)

18:10

Wolfgang Kemmetmüller (*TU Wien, Austria*)

Andreas Kugi (*TU Wien, Austria*)

Injection molding is one of the most important manufacturing processes in the polymer industry. While extruder machines are working in continuous operation, the injection molding process typically is a non-continuous but cyclic process. This cyclic process consists of the following phases: closing the mold, filling of the mold with molten polymer, packing, cooling, plastication, and ejection of the final part.

An accurate control of the process variables (e.g. injection pressure and speed) to their desired values (in particular during the filling and packing phase) is essential to obtain a constant high product quality. In [1], a control-oriented first-principles model of the filling and packing phase was introduced, which is the basis for a nonlinear model-predictive control (MPC) concept presented in [2]. Since there is typically only very limited knowledge of the mold when the controller is designed the volume flow into the mold has to be estimated online. The control concept presented in [2] utilizes measurements of the current injection cycle only. As the injection molding process is a cyclic batch process it seems meaningful to additionally use information from the previous cycle.

In the present work, an identification method for the volume flow into the mold is developed by analyzing the entire last injection cycle. The method exploits the advantages of non-causal filters, which entail an improved estimation accuracy of the volume flow over the whole cycle compared to an online estimation. The estimations of the previous cycles are then utilized in an online two-degrees-of-freedom estimator concept. It combines the advantages of the high accuracy of the offline estimations with the capability to account for variations of the injection process by an online estimation. Given the offline estimations of the previous cycles, a prediction of the volume flow within the MPC prediction horizon allows to react on future changes of the mold behavior. The proposed method in combination with the MPC is validated by detailed simulation studies, which show a significant improvement of the control performance compared to MPC without the cycle-based adaption.

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S20.06 | Dynamics and control

Date: February 21, 2019

08:30-10:30

Room: HS 05

Optimal periodic control of nonlinear chemical reactions with a time-varying flow rate

Alexander Zuyev (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany, National Academy of Sciences of Ukraine, Ukraine*) 08:30

Andreas Seidel-Morgenstern (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

This presentation deals with a mathematical model of a non-isothermal chemical reaction described by nonlinear ordinary differential equations with two-dimensional control. The control variables correspond to the possibility of manipulating the concentration of the input reactant and the total flow rate. The performance of such reactions has been analyzed in [1] by the nonlinear frequency response method with one sinusoidal input. In the present work, we consider the case of two independent inputs and treat the task of maximizing the reactor performance as an isoperimetric optimal control problem with periodic boundary conditions. This problem formulation differs from the previous paper [2] as the integrand of the cost depends on the state, and the system under consideration is not control-affine. We analyze necessary optimality conditions by the Pontryagin maximum principle and propose estimates of the number of switchings for extremal controls. We take into account the isoperimetric constraints by introducing Lagrange multipliers in the Hamiltonian of the considered problem. Then periodic extremal trajectories are constructed analytically by exploiting the Fliess functional expansion. We evaluate the cost for these trajectories and solve the resulting finite-dimensional optimization problem with respect to the switching parameters to find optimal phases for the input signal. Conditions for improving the reactor performance in comparison to its steady-state operation are derived analytically and illustrated with numerical simulations. We also compare these results with the study of reactors controlled by modulating the inlet temperature and concentration under a constant flow rate.

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Optimal control of district heating systems

Dominik Linn (*Fraunhofer ITWM, Germany*) 08:50

Jan Mohring (*Fraunhofer ITWM, Germany*)

Norbert Siedow (*Fraunhofer ITWM, Germany*)

For the purpose of reducing the emissions of greenhouse gases, the concept of integrated energy systems has emerged. A special role is taken by district heating systems, as they can use excess heat from other processes, such as the generation of electric energy. Furthermore, their inherent time delay behavior allows for a temporal decoupling, which unlocks further potential for optimization.

Within the scope of the project “DYNEEF”, funded by the BMWI, we focus on the mathematical modelling and optimal control of district heating systems, where ecological, and economic constraints, as well as integration with other energy systems have to be considered.

Typical models for network components and coupling conditions naturally lead to a system of nonlinear algebraic and hyperbolic partial differential equations, which serve as constraints within the optimal control problem. Major difficulties arise from the large number of algebraic constraints, and the necessity for a long-time prediction horizon. It has shown to be beneficial to make use of the already known analytical solution for individual network components (van der Heijde et al. [1]). We extend this approach to an implicit, semi-analytical scheme, which allows for a efficient, combined solution of the algebraic and partial differential equations. In order to integrate the numerical forward simulation with an optimal control problem, we make use of automatic differentiation (see [2]). Thereby, we sequentially solve the system’s dynamic equations and simultaneously compute piecewise linearizations of the cost functional, and inequality constraints, which results in a quadratic optimization problem.

Finally, we present an application of our method to a model problem for an existing district heating network.

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Coordinate-invariant linear quadratic control

Ethan R. Burnett (*University of Colorado Boulder, United States of America*) 09:10

Andrew James Sinclair (*Air Force Research Laboratory, United States of America*)

Eric A. Butcher (*University of Arizona, United States of America*)

A given physical system can generally be described by a variety of coordinate choices, each of which satisfies a set of nonlinear equations of motion. It is well understood that the solutions for these coordinates share an equivalence, simply being different representations of the same dynamics, and are related by nonlinear coordinate transformations. However, different coordinate choices can vary greatly in convenience, the level of insight they provide, and significantly, the amount of nonlinearity in their equations of motion. To help analyze the available representations for a given physical system, a nonlinearity index has been developed to analyze the nonlinearity of a specific coordinate representation.

Due to the difficulty in working with nonlinear equations of motion, linear approximations are often used. One of the foundational techniques for control of dynamical systems is linear quadratic regulation (LQR), which are designed based on linear approximations of the equations of motion. In applying this technique, it is broadly believed that selecting coordinates with low values of nonlinearity will provide better performance.

Recent discoveries have demonstrated the equivalence of the linearized approximations for various coordinate representations, being related by the linearized coordinate transformations. Additionally, a calibration process, making judicious use of the nonlinear and linearized coordinate transformations, has been developed to generate more accurate approximations of highly nonlinear coordinates. This paper will demonstrate how the calibration process can be used to improve the LQR control performance for highly nonlinear coordinates.

The LQR design process for a given set of coordinates involves linearly approximating the equations of motion, solving the associated Riccati equation, and computing the control gain. For

two different coordinate choices, this paper will demonstrate the mapping between the solutions of the two Riccati equations, and demonstrate how the mapping between the resulting control gains. This shows that control performance associated with a less nonlinear coordinate choice can be reconstructed by applying the calibration process to the LQR controller designed for a highly nonlinear coordinate choice. Preliminary results have shown that the calibration process can improve the performance of LQR control methods and expand the domain of convergence by orders of magnitude.

Adjoint sensitivity equations in optimal control of differential-algebraic equations

Daniel Bankmann (*TU Berlin, Germany*)

09:30

Optimal control problems for differential-algebraic equations appear in a variety of applications coming from electrical or mechanical engineering.

Sometimes, the system's descriptions are also depending on parameters and one is not only interested in computing the solution of such a problem. In addition, we are interested in computing how the solution changes for small changes in the parameters, i. e. the sensitivities of the optimal solution with respect to the parameters.

Solutions of the optimal control problem can be characterized by so-called necessary conditions. These constitute a boundary value problem for differential-algebraic equations.

In the current literature, only sensitivity analysis for initial value problems of differential-algebraic equations or boundary value problems for ordinary differential equations has been carried out, although theory for adjoint equations with boundary values exists.

We close this gap, by formulating the correct boundary conditions based on the standard adjoint equations for differential-algebraic equations of d-index 1 in the framework of the strangeness index. This includes jump conditions on certain variables which pose challenges on solvability and existence of solutions.

In this talk, we present an adjoint sensitivity boundary value problem for d-index 1 differential-algebraic equations with boundary values. Based on a flow formulation, we analyze properties like existence and uniqueness and apply these results to the necessary conditions coming from the optimal control problem. We also discuss possible solutions for tackling resulting numerical issues.

Optimal feed forward control of hydraulic drive systems with long pipelines

Christopher Pietschnig (*TU Wien, Austria*)

09:50

Lukas Marko (*TU Wien, Austria*)

Wolfgang Kemmetmüller (*TU Wien, Austria*)

Andreas Kugi (*TU Wien, Austria*)

Hydraulic drive systems are widely used in technical applications, ranging from the automotive and aerospace sector to industrial production processes. They yield high forces and torques for long distances and high speeds at a compact design. The typical setup of hydraulic drive systems comprises a valve which is used to control a hydraulic cylinder or motor. In many practical applications, the valve is connected to the hydraulic cylinder via hydraulic pipelines, whose length can amount for several meters. In current force or position control concepts, the influence of these pipelines is typically neglected. During fast operation of the hydraulic drive systems, wave effects can be excited, which significantly deteriorate the control performance up to instability of the closed-loop system. Thus, the controllers have to be tuned sufficiently slow to circumvent this problem.

The behavior of hydraulic pipelines is well described by a set of partial differential equations [1]. The state-of-the-art approach for spatial discretization of these equations is the method of

characteristics (MOC). This procedure results in a high number of states and is therefore not well suited for model-based controller design. In this work, the spectral elemental method (SEM) is applied [2], which exhibits a similar accuracy as the MOC with a significantly lower number of states. Based on such a SEM-model, an optimal feed forward control strategy is developed for a hydraulic drive system with long pipelines. The proposed approach allows to systematically consider actuator constraints and to compensate the wave effects introduced by the hydraulic pipelines. The optimal control problem is efficiently solved on a moving horizon, which serves as the basis for the design of a real-time capable moving horizon trajectory planning strategy. The behavior and the high potential of the proposed approach is demonstrated by simulation studies. In particular, it is shown that the systematic consideration of the actuator constraints and the dynamics of the hydraulic pipelines enables smooth and fast set-point changes.

[1] E. B. Wylie and V. L. Streeter, Fluid transients in Systems. Prentice Hall Englewood Cliffs, USA, 1993.

[2] J.-F. Mennemann, L. Marko, J. Schmidt, W. Kemmetmüller, and A. Kugi, "The spectral element method as an efficient tool for transient simulations of hydraulic systems," Applied Mathematical Modelling, vol. 54, pp. 627-647, 2018.

Feedback and feedforward control concepts to improve road holding for passenger cars

Florian Klinger (*TU Wien, Austria*)

10:10

Johannes Edelmann (*TU Wien, Austria*)

Manfred Plöchl (*TU Wien, Austria*)

In recent years, semi-active suspension systems have become a standard in premium class automobiles. "Sky-hook damping" has been suggested in literature, as well as a "ground-hook" approach to minimize road damage for commercial vehicles and to improve road holding for passenger cars. However, knowledge on the actual road unevenness velocity is needed, since the tyre vertical deflection speed is included in the control law, and numerical optimization is proposed to tune respective controller parameters. In this study, an optimal control will be presented that includes the actual road unevenness velocity by means of disturbance feedforward. Thus, advantages of the ground-hook control can be retained. The proposed control law combines disturbance feedforward and full state-vector feedback control, keeping benefits and ease of LQ control design. In addition, interpretation of the control law reveals the opportunity to systematically separate effects of the feedback and feedforward gains on the performance measures. Simulation results will be presented based on a quarter-car model.

S20.07 | Dynamics and control

Date: February 21, 2019

14:00-16:00

Room: HS 05

Extensions of a standard iterative learning control framework and their relevance for a range of applications

Thomas Seel (*TU Berlin, Germany*)

14:00

Iterative Learning Control Theory has first been proposed almost 35 years ago to improve performance in control tasks that repeat in trials. Since then a number of algorithms and frameworks have been developed and were successfully applied to electromechanical systems with strong repetitiveness. More recently, large research efforts have been made to overcome some of the fundamental limitations of standard learning control theory including assumptions on uniform trial duration, trial-invariant initial conditions, and lossless communication. This results in new methods that can be applied to a larger range of applications in energy systems, process automation, autonomous systems, and biomedical engineering. This talk provides an introduction to a standard Iterative Learning Control framework, an overview of significant extensions of that framework, a demonstration of the control performance achieved in several application systems, and a discussion of open problems.

Differences and similarities between reinforcement learning and the classical optimal control framework

Simon Gottschalk (*Fraunhofer ITWM, Germany*)

14:40

Michael Burger (*Fraunhofer ITWM, Germany*)

In this talk, we focus on reinforcement learning (RL) in order to control dynamical systems. We will introduce the idea and structure of RL and point out the similarities between RL and classical techniques to solve optimal control problems. Despite the similarities, major differences such as the closed-loop- instead of the open-loop-optimization exist. We will discuss, for which kind of problem or task, RL is beneficial and which techniques are worth investigating. Furthermore, we analyze a model-free, policy-based RL algorithm based on neural networks and we apply it in two different settings: biomechanical system like a muscle actuated arm and a robot in an assembly process.

A combined homotopy-optimization approach to parameter identification for dynamical systems

Kai Schäfer (*University of Bremen, Germany*)

15:00

Kathrin Flaßkamp (*University of Bremen, Germany*)

Jörg Fliege (*University of Southampton, United Kingdom*)

Christof Büskens (*University of Bremen, Germany*)

The identification of parameters in dynamic systems plays an important role in many engineering processes. Although there exist sophisticated methods like direct multiple shooting algorithms, the single shooting approach is still widely used. One of the main challenges in parameter identification is to overcome being stuck in local optima instead of finding the global one. Therefore, Vyasarayani et al. [1] propose to use a specific homotopy formulation, in which the dynamics are

augmented by an observer term in combination with a homotopy parameter. By repeatedly solving the proposed problem formulation with linearly decreasing homotopy values, global minima can be attained in several numerical examples.

We modify this approach by embedding the continuation process into a more general nonlinear optimization framework, which allows for the choice of more efficient homotopy paths. In particular, we treat the homotopy parameter as an optimization variable. By initializing it sufficiently large and by adding a penalty term to the objective function, we obtain an equivalent problem formulation. In contrast to [1], the optimization problem has to be solved only once.

With the help of academic numerical examples we demonstrate that this extended approach is beneficial regarding both solution quality and efficiency. The problems are solved by the NLP solver WORHP [2].

[1] C. P. Vyasarayani, T. Uchida, and J. McPhee. Nonlinear parameter identification in multi-body systems using homotopy continuation. *Journal of Computational and Nonlinear Dynamics*, 7/1, American Society of Mechanical Engineers, 2012.

[2] C. Büskens and D. Wassel. *The ESA NLP solver WORHP. Modeling and optimization in space engineering*, Springer, 2012.

S21 | Mathematical signal and image processing

Organiser: Otmar Scherzer (*University of Vienna, Austria*)
Gwenael Mercier (*University of Vienna, Austria*)
Clemens Kirisits (*University of Vienna, Austria*)

S21.01 | Mathematical signal and image processing

Date: February 20, 2019
Room: SR 02

16:30-18:30

Numerical algorithms for stabilised backward image evolutions

Joachim Weickert (*Saarland University, Germany*) 16:30
Martin Welk (*UMIT, Austria*)
Leif Bergerhoff (*Saarland University, Germany*)
Marcelo Cardenas (*Saarland University, Germany*)
Guy Gilboa (*Technion, Israel*)

Backward parabolic differential equations are potentially useful for image enhancement and deblurring. However, these processes are ill-posed and suffer from intrinsic instabilities. These difficulties have prevented many researchers from using backward evolutions. The goal of this talk is to show that this fear is unsubstantiated, provided that one supplements the models with suitable stabilisation techniques and takes care that the numerical algorithms reproduce all qualitative properties of the continuous models in an adequate way. Prototypical models include forward-backward diffusion processes and repulsive particle systems with range constraints.

Riemannian structure and flows for smooth geometric image labeling

Fabrizio Savarino (*Heidelberg University, Germany*) 17:10
Christoph Schnörr (*Heidelberg University, Germany*)

The image labeling problem can be described as assigning to each pixel a single element from a finite set of predefined labels. Recently, a smooth geometric approach for inferring such label assignments was proposed by following the Riemannian gradient flow of a given objective function on the so-called assignment manifold. Due to the specific Riemannian structure, this results in a coupled replicator dynamic incorporating local spatial geometric averages of lifted data-dependent distances. However, in this framework an approximation of the flow is necessary in order to arrive at explicit formulas. We discuss preliminary results of an alternative model where lifting and averaging is decoupled in the objective function so as to stay closer to established approaches and at the same time preserve the ingredients of the original approach. As a consequence the resulting flow is explicitly given, without the need for any approximation, while still exploiting the underlying Riemannian structure.

Geometric numerical integration of the assignment flow

Alexander Zeilmann (*Heidelberg University, Germany*) 17:30
Fabrizio Savarino (*Heidelberg University, Germany*)
Stefania Petra (*Heidelberg University, Germany*)
Christoph Schnörr (*Heidelberg University, Germany*)

The assignment flow is a smooth dynamical system that evolves on an elementary statistical manifold and performs contextual data labeling on a graph. We derive and introduce the linear assignment flow that evolves nonlinearly on the manifold, but is governed by a linear ODE on the tangent space. Various numerical schemes adapted to the mathematical structure of these two models are designed and studied, for the geometric numerical integration of both flows: embedded Runge-Kutta-Munthe-Kaas schemes for the nonlinear flow, adaptive Runge-Kutta schemes and exponential integrators for the linear flow. All algorithms are parameter free, except for setting a tolerance value that specifies adaptive step size selection by monitoring the local integration error, or fixing the dimension of the Krylov subspace approximation.

Generalised quantiles for multivariate images

Martin Welk (*UMIT, Austria*)

17:50

For robust local filtering of multivariate images, generalisations of filters for scalar images based on robust statistical measures are an important approach. In past work, we have investigated several multivariate median concepts from statistics literature, focusing on their applicability and properties in an image processing context, including PDE approximations in the space-continuous limit. For the concept of quantiles, generalisations to multivariate data are possible; instead of an interval the position parameter comes from a unit ball in the data space. We investigate multivariate quantile concepts related to several multivariate median concepts and explore their possible use as robust image filters.

A method for image decomposition and particle quantification

Stefan Günther (*TU Dresden, Germany*)

18:10

Stefan Odenbach (*TU Dresden, Germany*)

Investigations using micro X-ray tomography are an outstandingly suitable experimental approach to analyze deep bed filtration processes. The three-dimensional images of model filters provide information about the filter bed structure, as well as the locations of the deposited particles. Small particles with a size about 1 micron are of particular interest in these experiments.

In a model system with strongly absorbing molybdenum particles, they are clearly visible with high contrast, although they are significantly smaller as the resolution of the tomograms. Therefore, the particles cannot be quantified by simple thresholding. Furthermore the tomograms are noisy and show artifacts.

An image processing method will be presented, that consists of a sequence of basic operations and allows the decomposition of three-dimensional grey value images into the concentration distribution of the depicted materials. In the example of the filtration experiments these materials are glass as model filter, water respectively PU as replacement material, air and molybdenum particles.

Precondition for that method are normalized tomograms, wherein the certain materials are represented by the same grey value ranges. Furthermore the grey values for each material with the concentration $c = 1$ has to be determined in calibration measurements.

It is possible to determine in particular the particle distribution quantitatively with these image processing method. It was tested on different validation samples with well-known particle content and it could be shown for this model system, that they can be quantified with approx. $\pm 15\%$.

S21.02 | Mathematical signal and image processing

Date: February 21, 2019

08:30-10:30

Room: SR 02

Deblurring and denoising using Tikhonov functionals with imperfect forward operators and epsilon-insensitive distances

Phil Gralla (*Stemmer Imaging, Germany*)

08:30

Iwona Piotrowska-Kurczewski (*University of Bremen, Germany*)

Peter Maass (*University of Bremen, Germany*)

Deblurring and denoising data can be described as solving an inverse problem. In this case the forward operator models the blurring effect and an appropriated regularization reduces the present noise. In application the true blurring model is rarely known. Instead an approximation or estimation has to be applied, which may add to the ill-posed nature of the inverse problem. In order to stabilize the inversion and allow for less perfect approximations in the forward model, we use ϵ -insensitive distances. These distances are known from support vector machines and we apply them to alter classic tikhonov functionals. Furthermore, we will consider various regularization terms and discuss the modelling and how to estimate the imperfect forward operator as well as numerical implementation of the inverse problem and its solver. Since standard solvers will not be sufficient for all considered noise models. In addition, a comparison to existing methods will be presented.

Musical instrument separation on shift-invariant spectrograms via stochastic dictionary learning

Sören Schulze (*University of Bremen, Germany*)

08:50

Emily J. King (*University of Bremen, Germany*)

We propose a novel method for the blind separation of audio signals produced by musical instruments. While the approach of applying non-negative matrix factorization (NMF) has been studied in many papers, it does not make use of the pitch-invariance that the sounds of instruments exhibit. This limitation can be overcome by using tensor factorization, in which context the use of log-frequency spectrograms was initiated, but this still requires the specific tuning of the instruments to be hard-coded into the algorithm. We develop a time-frequency representation that is both shift-invariant and frequency-aligned, with a variant that can also be used for wide-band signals. Our separation algorithm exploits this shift-invariance in order to find patterns of peaks related to specific instruments, while non-linear optimization enables it to represent arbitrary frequencies and incorporate inharmonicity, and the reasonability of the representation is ensured by a sparsity condition. The relative amplitudes of the harmonics are saved in a dictionary, which is trained via a modified version of ADAM. For a realistic monaural piece with acoustic recorder and violin, we achieve qualitatively good separation with a signal-to-distortion ratio (SDR) of 12.5 dB, a signal-to-interference ratio (SIR) of 26.1 dB, and a signal-to-artifacts ratio (SAR) of 12.7 dB, averaged.

Unsupervised Label Learning on Manifolds by Geometric Assignment

Artjom Zern (*Heidelberg University, Germany*)

09:10

Matthias Zisler (*Heidelberg University, Germany*)

Freddie Åström (*Heidelberg University, Germany*)

Stefania Petra (*Heidelberg University, Germany*)

Christoph Schnörr (*Heidelberg University, Germany*)

Manifold models of image features abound in computer vision. We present a novel approach that combines unsupervised computation of representative manifold-valued features, called labels, and the spatially regularized assignment of these labels to given manifold-valued data. Both processes evolve dynamically through two Riemannian gradient flows that are coupled. The representation of labels and assignment variables are kept separate, to enable the flexible application to various manifold data models. As a case study, we apply our approach to the unsupervised learning of covariance descriptors on the positive definite matrix manifold, through spatially regularized geometric assignment.

Extraction of wavefront sets by deep convolutional neural networks and shearlets

Hector Andrade Loarca (*TU Berlin, Germany*)

09:30

Gitta Kutyniok (*TU Berlin, Germany*)

Ozan Öktem (*KTH Stockholm, Sweden*)

Philipp Petersen (*University of Oxford, United Kingdom*)

The wavefront set is an important concept in distribution theory, in particular it generalizes the notion of singularities for distributions and characterizes their orientation. In multidimensional signal reconstruction the singularities of a signal and their orientations are often its most important features to reconstruct (e.g. Computed Tomography Reconstruction).

The main limitation implementing this concept faithfully in real-world applications resides in its abstract definition that depends strongly on the continuity of functional space, which makes it hard to algorithmically compute it in a digital setting. Multiscale systems such as wavelets or shearlets allow to extract the singularities of certain classes of functions. In addition the shearlet system also allows to compute the orientation of such singularities and therefore the wavefront set of the function under study.

In this talk we will address the particular limitations when trying to define the wavefront set on digital signals and design analytically an algorithm to extract it. We will then present an algorithmic approach based on a carefully designed convolutional neural network which uses the shearlet transform of an image to extract its wavefront set in form of its edges and orientations. Our method outperforms the well known state-of-the-art Wavefront Set Extractors including the ones using a Deep Learning approach.

The mismatch principle: statistical learning under large model uncertainties

Martin Genzel (*Technische Universität Berlin, Germany*)

09:50

Gitta Kutyniok (*Technische Universität Berlin, Germany*)

We study the learning capacity of the generalized Lasso with an arbitrary convex constraint set. While these types of estimators were originally designed for noisy linear regression problems, it recently turned out that they are in fact capable of handling considerably more complicated situations, involving highly non-linear distortions. This talk intends to provide a comprehensive explanation of this somewhat astonishing phenomenon. At the heart of our analysis stands the mismatch principle, which is a simple, yet generic recipe to establish theoretical error bounds for empirical risk minimization. The scope of our results is fairly general, permitting arbitrary sub-Gaussian input-output pairs, possibly with strongly correlated feature variables. Noteworthy, the mismatch principle also generalizes to a certain extent the classical orthogonality principle for ordinary least squares. This adaptation allows us to investigate problem setups of recent interest, most importantly, high-dimensional parameter regimes and non-linear observation processes. In particular, our theoretical framework is applied to various scenarios of practical relevance, such as single-index models, variable selection, and strongly correlated designs. We thereby demonstrate

the key purpose of the mismatch principle, that is, learning (semi-)parametric output rules under large model uncertainties and misspecifications.

Dimension reduction in learning tasks

Anna Breger (*University of Vienna, Austria*)

10:10

Martin Ehler (*University of Vienna, Austria*)

Bianca S. Gerendas (*Medical University of Vienna, Austria*)

Jose Ignacio Orlando (*Medical University of Vienna, Austria*)

Ursula Schmidt-Erfurth (*Medical University of Vienna, Austria*)

Motivated by the analysis of biomedical imaging data, we shall discuss the use of dimension reduction in combination with standard learning tools. Orthogonal projections are a powerful analysis tool to emphasize specific data features and at the same time reduce the overall complexity simplifying further processing. The underlying objective in the use of random projections is the preservation of relative pairwise distances, theoretically supported by the famous Johnson-Lindenstrauss-Lemma. Principal component analysis (PCA), on the other hand, identifies an orthogonal projector that maximizes the total variance. We observe that the scaled preservation of relative pairwise distances and the maximization of the total variance are competing objectives, in particular, in high dimensions. Therefore, the specific choice of the orthogonal projection used for subsequent analysis is critical and highly depends on the data and the learning task. Besides the specific architecture, iterative learning frameworks usually depend on a loss function to quantify residuals in intermediate steps. We introduce variational loss functions based on orthogonal projections to integrate and emphasize target information. These variational loss functions are applied in a medical image classification problem, where the overall task is the classification of photoreceptor layers and their disruptions in the human retina. Optical coherence tomography scans with binary pixel-wise annotations by retinal specialists allow analysis in a supervised manner with deep convolutional neural networks. Optimizing standard loss functions does not sufficiently identify disruptions, whereas the use of our proposed variational loss function can improve the detection.

S21.03 | Mathematical signal and image processing

Date: February 21, 2019

14:00-16:00

Room: SR 06

Mathematical challenges of correspondence problems

Jan Modersitzki (*University of Lübeck, Germany*)

14:00

An overview of state-of-the-art image registration techniques is presented. Image registration or correspondence problems are one of the big challenges in imaging, particularly in medical imaging. Roughly speaking, the goal is to automatically establish geometrical correspondences between structures in images.

Although this problem appears in presumably every imaging area, we focus on applications from medical imaging. The talk presents a variety of examples such as the reconstruction of a histological serial sectioning, the correction of motion artefacts, the determination of changes with respect to a baseline, or the fusion of data, where information from different sensors is to be combined.

Mathematically, image registration is an ill-posed problem and therefore a variational framework is facilitated that optimizes an objective functional with a data-fit and a regularization. The ill-posedness can readily be deduced from the fact vector is to be determined from a given

scalar. Moreover, constant areas can be rearranged arbitrarily without changing the image interpretation.

Models for data-fits are presented and discussed. In particular, we present a new Schatten- q -norm based measure designed for time series of images. Roughly speaking the idea is to minimize the rank of a matrix formed of image gradients. For low rank, the gradients and hence the images are aligned. In contrast to standard approaches, the new measure is based on the whole sequence. We discuss various regularizers including parameterized spaces, quadratic energies, non-convex energies as well as velocity constrained approaches, the so called large deformation diffeomorphic metric mappings (LDDMM). The necessary conditions for a minimizing element is interpreted as a balance of forces, where the outer forces generated by the data-fit have to match the internal forces specified by the regularizer. This interpretation indicates that a proper choice of regularization is not just a mathematical issue but also requires an understanding of the underlying data source.

For many applications, the mathematical approach outlined above is insufficient to produce meaningful i.e. application conform solutions. Constraints on the transformation space can lead to more realistic solutions. Examples of constraints include prescribed point correspondences, bounds on volume changes, local rigidity, or region matching.

The talk will close with an outlook. Although the mathematical theory is well-established for unconstrained registration, too little is known for the constrained setting. For example, local rigidity constraints it has been observed that first order regularizer yield displeasing results on the interfaces whereas a hyperelastic energies yields much smoother transformation across the interfaces.

Improved edge detection based on fractional derivatives for real-time measurement systems

Maximilian Loderer (*Technische Universität Dresden, Germany*)

14:40

Michael Beitelschmidt (*Technische Universität Dresden, Germany*)

The increasing urbanization demands modern light rail vehicles with great passenger capacity as well as high transportation comfort, to increase the attractiveness of public transport and thus reduce traffic.

The Chair of Dynamics and Mechanism Design of the TU Dresden has developed a real-time measuring system for light rail vehicles to record the track geometry and position as well as the clearance gauge during regular carriageway operation. The measured data can be used for an improved design of new light rail vehicles. Within the scope of the research project, there is a need for robust edge detection algorithms for the rail detection from camera data in real time.

As part of the development project, a new edge detection approach was proposed by C. Telke using fractional derivatives called eCRONE (extended Contour Robust d'Ordre Non Entier). The proposed real-time algorithm detects edges of changing contrast within gray-scale images, especially perpendicular to the search direction. The proposed approach is characterized by a robust detection in the presence of high noise. Disadvantages are the anisotropy of the filter and, in comparison to reference methods, smearing of the detected edge.

To overcome these disadvantages a development of the eCRONE, the novel Operator rCRONE (radial Contour Robust d'Ordre Non Entier) is proposed.

Instead of joining CRONE vectors together to form a matrix, the eCRONE, every entry of the rCRONE matrix is calculated with respect to its distance and angle to the anchor of the filter kernel. Although this filter is still directional, the fractional derivatives on the interval of $(-90, 90)$, locally considered, are equally included.

In a benchmark study it can be shown that the new proposed rCRONE filter can detect edges in a higher resolution and much more accurately in presence of high noise compared to the

former eCRONE. However, the required computational effort does not increase. Furthermore, the rCRONE allows a much better detection of curves and sloping lines, so that it can also be applied in the image recognition in presence of noisy input data. The contribution explains the theory of the new filter and presents the benchmark study.

Solving bilinear and quadratic inverse problems using tensorial liftings

Robert Beinert (*Karl-Franzens-Universität Graz, Austria*)

15:00

Bilinear and quadratic inverse problems arise in various formulations in imaging and physics like blind deconvolution, deautoconvolution, parallel imaging in MRI, or phase retrieval. Although the corresponding forward operators in the problem formulation are only slightly non-linear, in many instances, the requirements to apply the well-established non-linear regularization theory are not fulfilled.

In this talk, we show that the essential results of the classical regularization theory with bounded linear operators and convex regularization functionals can nevertheless be extended to bilinear and quadratic forward operators. At the same time, we allow the regularization functional to be non-convex in a manner being comparable with the non-linearity of the considered operators. The central idea to establish a regularization theory for bilinear and quadratic operators is here the universal property of the topological tensor product, which enables us to lift the considered forward operators to linear mappings. Owing to the lifting, we get immediate access to the linear regularization theory. On the down-side, a simple lifting of the non-linear inverse problem causes an additional non-convex rank-one constraint, which is similarly challenging to handle than the original non-linear problem. For this reason, most results of the linear regularization theory are not applicable for the lifted problem and cannot be transferred to the original (unlifted) inverse problem.

In order to overcome this issues, we use the tensorial lifting indirectly and generalize the required concepts like subdifferentials and Bregman distances from convex analysis to the new framework. Using a source-wise representation as in the classical range condition, we derive convergence rates for the regularized solutions with respect to the actual noise level. Finally, we apply our results to problem formulations in signal processing to derive satisfiable source conditions and numerically provable convergence rates.

Dynamical super-resolution with applications to ultrafast ultrasound imaging

Francisco Romero Hinrichsen (*University of Graz, Austria*)

15:20

Habib Ammari (*ETH Zurich, Switzerland*)

Giovanni Alberti (*University of Geona, Italy*)

Timothée Wintz (*ENS Paris, France*)

Recently there has been a successful development in ultrasound imaging, increasing significantly the sampling rate and therefore enhancing this imaging's capacities. In particular, for vessel imaging, the use of microbubble tracking allows us to super-resolve blood vessels, and by estimating the particles' speeds inside them, it is possible to calculate the vessels' diameters. In this context, we model the microbubble tracking problem, formulating it in terms of a sparse spike recovery problem in the phase space (the position and velocity space), that allows us to obtain simultaneously the speed of the microbubbles and their location. This leads to an L1 minimization algorithm for point source tracking, that promises to be faster than current alternatives.

A clustering algorithm for single-molecule localization in super-resolution microscopy

Patrick Günther Schneider (*TU Vienna, Austria*)

15:40

Magdalena Schneider (*TU Vienna, Austria*)

Gerhard Schütz (*TU Vienna, Austria*)

Clemens Heitzinger (*TU Vienna, Austria*)

In Super-Resolution Microscopy, the complex blinking behaviour of fluorescent chemical compounds is an issue in the process of identification and localisation of single molecules. Common clustering methods lead to unsatisfactory results for these kind of data and demand further development under the constraint to perform fully automatically without additional input besides the experimental data. The measurements arise from a large number of single-image frames (in this study 10,000 frames). Data are provided as postprocessed dSTORM output files after noise reduction and rough prior adjustment. The rows of such output files contain information associated with a single blinking event, and the columns used are frame number, x-coordinate, and y-coordinate. We have developed a clustering algorithm based on merging clusters using the Kullback-Leibler Divergence (KLD). The model transforms given data into a composition of multivariate normal distributions, which allows first-hand application of the Kullback-Leibler Divergence when calculating distances between clusters. The KL-clustering algorithm proceeds based on a prescribed minimum threshold α . A K-component multivariate normal distribution is collapsed into a (K-1)-component model until the minimum KLD of the mixture components has reached the threshold α . Since we have no a priori information about the optimal value for α , we execute the clustering algorithm for a certain interval (α_{\min} , α_{\max}), which is computed based on quantiles of the frame statistics. Comparing elements from such a list of α -dependent distributions based on the rate of change of the corresponding likelihood functions allows model selection in a way similar to dendrogram analysis in hierarchical clustering. Moreover, since the blinking of single molecules is clustered in time, all calculations in the clustering algorithm are performed in the three-dimensional space (frame number, x, y), which takes the complex time-dependent blinking behavior of the single molecules into account. Furthermore, numerical results show that a transformation of the frame variable based on histogram statistics of observations leads to better results than simple linear or log scaling. Therefore we chose a fitted geometric distribution based on the MLE for the histogram data and transformation of frame values into their pmf value for said geometric distribution. Numerical results for the challenging case of clustered molecules with few blinking events show that the calculated number of molecules agrees very well with the true number of molecules when using a threshold value α as calculated above.

S21.04 | Mathematical signal and image processing

Date: February 21, 2019

17:40-18:40

Room: SR 06

On the robust PCA and Weiszfeld's algorithm

Sebastian Neumayer (*Technische Universität Kaiserslautern, Germany*)

17:40

Max Nimmer (*Technische Universität Kaiserslautern, Germany*)

Simon Setzer (*Engineers Gate, United Kingdom*)

Gabriele Steidl (*Technische Universität Kaiserslautern, Germany, Fraunhofer ITWM, Germany*)

Principal component analysis (PCA) is a powerful standard tool for reducing the dimensionality of data. Unfortunately, it is sensitive to outliers so that various robust PCA variants were proposed in the literature. This paper addresses the robust PCA by successively determining the directions of lines having minimal Euclidean distances from the data points. The corresponding energy functional is not differentiable at a finite number of directions which we call anchor directions. We derive a Weiszfeld-like algorithm for minimizing the energy functional which has several advantages over existing algorithms. Special attention is paid to the careful handling of the anchor directions, where we take the relation between local minima and one-sided derivatives of Lipschitz continuous functions on submanifolds of R^d into account. Using ideas for stabilizing the classical Weiszfeld algorithm at anchor points and the Kurdyka-Łojasiewicz property of the energy functional, we prove global convergence of the whole sequence of iterates generated by the algorithm to a critical point of the energy functional. Numerical examples demonstrate the very good performance of our algorithm.

Reconstruction of non-stationary signals by the generalized Prony method

Gerlind Plonka (*Georg-August Universität Göttingen, Germany*)

18:00

Kilian Stampfer (*Georg-August Universität Göttingen, Germany*)

Ingeborg Keller (*Georg-August Universität Göttingen, Germany*)

Peter & Plonka(2013, Inverse Problems 29) derived a generalized Prony method for the reconstruction of sparse expansions of eigenfunctions of suitable linear operators using only a small number of suitable sample values. Although some examples were given by Peter & Plonka the problem of finding such operators is non-trivial. In this talk we look at different generalizations of shift operators and their corresponding sets of eigenfunctions and eigenvalues that admit a reconstruction of structured functions from function values. In particular, we present a way to use these operators in order to reconstruct signal models such as arbitrary linear combinations of Gaussians, Gabor expansions with a Gaussian window as well as non-stationary trigonometric expansions with a special monotone phase function via the generalized Prony method.

K. Stampfer, G. Plonka and I. Keller Reconstruction of stationary and non-stationary signals by the generalized Prony method Analysis and Applications, to appear, 2018.

S21.05 | Mathematical signal and image processing

Date: February 22, 2019

08:30-10:30

Room: SR 06

Total variation based Lavrentiev regularisation for signal processing

Markus Grasmair (*NTNU, Norway*)

08:30

We will consider the solution of deconvolution problems in signal processing with noisy measurements. If we assume the true signal to be piecewise constant, then total variation regularisation with appropriately chosen regularisation parameter produces good and reliable results. However, the solution of the resulting variational problem requires the whole signal as input data, which precludes its usage for real time computations. In this talk, we will present an alternative that is based on the idea of Lavrentiev regularisation, again with a total variation like regularisation term. After discussing the basics of this method, we will introduce a numerical solution algorithm that preserves the structure of the deconvolution problem and can be essentially implemented in real time.

A convex variational model for learning image descriptors from incomplete data

Antonin Chambolle (*Ecole Polytechnique, France*)

08:50

Martin Holler (*University of Graz, Austria*)

Thomas Pock (*Graz University of Technology, Austria*)

We present and analyze a variational model for learning image descriptors from corrupted and/or incomplete data, both in function space and numerically. Building on lifting and relaxation strategies, the proposed approach is convex and allows for simultaneous image reconstruction and descriptor learning in a general, inverse problems context. Further, motivated by an improved numerical performance, we also discuss a semi-convex variant of the proposed model. For both settings, fundamental analytical properties allowing in particular to ensure well-posedness and stability results for inverse problems are derived in a continuous setting. Exploiting convexity, we further show numerical results where globally optimal minimizers of the proposed energy are computed for applications with incomplete, noisy and blurry data.

Sparsity of solutions for variational inverse problems with finite-dimensional data

Kristian Bredies (*Karl-Franzens-Universität Graz, Austria*)

09:10

Marcello Carioni (*Karl-Franzens-Universität Graz, Austria*)

In this contribution we characterize sparse minimizers of variational inverse problems of the form $R(u) + F(Au)$, where A is a linear continuous operator that maps into a finite dimensional Hilbert space, R is a seminorm and F is a convex functional. More precisely we prove that there exists a minimizer that is "sparse" in the sense that it is represented as a linear combination of the extremal points of the unit ball of the regularizer (possibly translated by an element in the null space of R).

Then we apply this result to relevant examples. First we consider the BV seminorm as a regularizer and we characterize the extremal points of its unit ball (extending a result of Ambrosio, Caselles, Masnou and Morel), giving a theoretical justification of the staircase effect typical of the TV regularization in image denoising. As a second application we consider the Radon norm

of linear, scalar differential operator. Our abstract result applies to this case when we consider as a minimization domain the distributions of finite order endowed with the weak* topology. Using this setting we recover a recent result of Unser, Fageot, Ward under weaker hypotheses. This is a joint work with Kristian Bredies.

Convergent domain decomposition methods for total variation minimization

Andreas Langer (*University of Stuttgart, Germany*)

09:30

Total variation regularisation is an important tool to solve inverse imaging problems. In particular, in the last decades, in the literature, there have been introduced many different approaches and algorithms for minimizing the total variation. These standard techniques are iterative-sequentially formulated and therefore not able to solve large scale simulations in acceptable computational time. For such large problems we need to address methods that allow us to reduce the problem to a finite sequence of subproblems of a more manageable size, perhaps computed by one of the standard techniques. With this aim, we introduce domain decomposition methods for total variation minimization. The main idea of domain decomposition is to split the space of the initial problem into several smaller subspaces. By restricting the function to be minimized to the subspaces, a sequence of local problems, which may be solved easier and faster than the original problem, is constituted. Then the solution of the initial problem is obtained via the solutions of the local subproblems by glueing them together. In the case of domain decomposition for the non-smooth and non-additive total variation the crucial difficulty is the correct treatment of the interfaces of the domain decomposition patches. Due to the non-smoothness and non-additivity, one encounters additional difficulties in showing convergence of more general subspace correction strategies to global minimizers. In particular there do exist counterexamples indicating failure of splitting techniques. Nevertheless, in this talk we propose overlapping domain decomposition algorithms for the total variation minimization problem with the guarantee of convergence to a minimizer of the original functional. The analysis is based on the relation between the primal (original) total variation minimization problem and its (pre-)dual formulation. To the best of our knowledge, this is the first successful approach of a domain decomposition strategy for total variation minimization with a rigorous convergent analysis in an infinite dimensional setting. We provide numerical experiments, showing the successful application of the algorithms.

Joint reconstruction in multi-modal electron tomography

Richard Huber (*Karl Franzens University, Austria*)

09:50

Georg Haberfehlner (*Graz Centre for Electron Microscopy & Institute for Electron Microscopy and Nanoanalysis, Austria*)

Martin Holler (*Karl Franzens University, Austria*)

Gerald Kothleitner (*Graz Centre for Electron Microscopy & Institute for Electron Microscopy and Nanoanalysis, Austria*)

Kristian Bredies (*Karl Franzens University, Austria*)

In multi-modal electron tomography, tilt series of several signals such as X-ray spectra, electron energy-loss spectra, annular dark-field, or bright-field data are acquired at the same time in the transmission electron microscope and subsequently reconstructed in three dimensions. However, the acquired data often is incomplete, suffers from noise, and generally each signal is reconstructed independently of all other signals, not taking advantage of correlation between different datasets. This severely limits both resolution and validity of the reconstructed images. In this talk, we show how image quality in multi-modal electron tomography can be greatly improved by employing variational modeling and multi-channel regularization techniques [4]. To this aim, we employ a coupled Total Generalized Variation (TGV) [1,2] regularization that exploits correlation between

different channels. In contrast to other regularization methods, coupled TGV regularization allows to reconstruct both hard transitions and gradual changes inside each sample, and links different channels on the level of first and higher order derivatives. This favors similar interface positions for all reconstructions, thereby improving the image quality for all data, in particular for 3D elemental maps. The resulting optimization problem is solved using a primal-dual algorithm [3] for which we developed a parallel implementation on the Graphics Processing Unit, enabling 3D reconstructions in a timescale of minutes.

[1] Kristian Bredies. Recovering piecewise smooth multichannel images by minimization of convex functionals with total generalized variation penalty. In *Efficient Algorithms for Global Optimization Methods in Computer Vision - International Dagstuhl Seminar, Dagstuhl Castle, Germany, November 20-25, 2011, 2011 Revised Selected Papers*, pages 44-77.

[2] Kristian Bredies, Karl Kunisch, and Thomas Pock. Total Generalized Variation. *SIAM Journal on Imaging Science*, 3(3):492-526, 2010.

[3] Antonin Chambolle and Thomas Pock. A First-Order Primal-Dual Algorithm for Convex Problems with Applications to Imaging. *Journal of Mathematical Imaging Vision*, 40(1):120-145, 2011.

[4] Martin Holler, Richard Huber, and Florian Knoll. Coupled regularization with multiple data discrepancies. *Inverse Problems*, 34(8):084003, 2018.

S22 | Scientific computing

Organiser: Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)
Hartwig Anzt (*Karlsruhe Institute of Technology (KIT), Germany*)

S22.01 | Scientific computing

Date: February 19, 2019
Room: HS 42

08:30-10:30

Model order reduction for the masses

René Milk (*University of Münster, Germany*)

08:30

Petar Mlinarić (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Stephan Rave (*University of Münster, Germany*)

Felix Schindler (*University of Münster, Germany*)

By now, model order reduction (MOR) techniques such as Balanced Truncation, Krylov or Reduced Basis methods have been applied successfully to a variety of application problems modeled by ordinary or partial differential equations. These methods deliver very fast approximations of the input-to-output or parameter-to-output mapping of the given problem while rigorously controlling the approximation error. This makes MOR a valuable tool for multi-query applications like design optimization or simulations under constrained resources, e.g. on embedded systems. However, despite many success stories there is still a lack of MOR software solutions that can be effortlessly integrated into complex PDE simulation workflows without requiring expertise in MOR techniques.

After a brief introduction to MOR, I will introduce pyMOR (<https://www.pymor.org>), our own Python-based MOR software library, that has been built from ground up on an interface-based design to allow easy integration with various PDE-solver libraries, such as deal.II, DUNE, FEniCS or NGSolve. Besides a tour of pyMOR's features and some application examples, I will discuss the most important technical design choices behind pyMOR and the consequences of these choices for developers of MOR algorithms on the one hand and MOR end users on the other. Based on our experience with developing pyMOR, I will end my talk trying to answer what remains to be done to bring MOR to the masses and what the greater Scientific Computing community might learn from it. Moreover, I will give an outlook on our own current efforts to make pyMOR the go-to tool for all your MOR needs.

A-priori pole selection for reduced models in structural dynamics

Quirin Aumann (*Technical University of Munich, Germany*)

09:10

Gerhard Müller (*Technical University of Munich, Germany*)

Large models of complex dynamic systems can be evaluated efficiently using model order reduction methods. Many methods rely on a selection of expansion points (poles) prior to the reduction procedure, which can have a major impact on the quality of the resulting reduced model. In this contribution, we investigate methods to appropriately choose an initial set of expansion points for models discretizing structural dynamic problems.

For reducing the full model, the iterative rational Krylov algorithm (IRKA) is used, which finds an optimal reduced model for a given set of expansion points. To make an “educated guess”

about the location of the poles, the structure's geometry is examined. Based on the geometry, the total number of modes up to a certain frequency can be evaluated, as well as the number of modes in a specific frequency band using the one and two dimensional wave equations. Both numbers can be used to generate a set of initial expansion points: the total number of modes gives a hint to the minimum size of the reduced model, the modes per frequency band reveal the location of the poles. The latter can also be used to generate a reduced model approximating the full model only in a certain frequency range.

It will be evaluated, how IRKA performs in the proposed settings and how the a-priori choice of expansion points affects the convergence rate.

Parametric model order reduction using tensor principal orthogonal decomposition

Mikhail Pak (*Technical University of Munich, Germany*)

09:30

Maria Cruz Varona (*Technical University of Munich, Germany*)

Siyang Hu (*Jade University of Applied Sciences, Germany*)

Boris Lohmann (*Technical University of Munich, Germany*)

In this talk we will present tensor principal orthogonal decomposition (TPOD), a data-driven parametric model order reduction approach based on the multilinear singular value decomposition (MLSVD).

Similarly to the principal orthogonal decomposition (POD), TPOD requires that a full order model be simulated with different parameter sample values. The obtained state trajectory snapshots are then organized in a snapshot tensor such that the state-space variables are arranged along the first and the simulation time steps along the second mode. Third and higher modes of the snapshot tensor represent the variation along the respective parameter sample values.

This snapshot tensor is subsequently decomposed using the MLSVD into a core tensor and at least three factor matrices: A state-space basis factor matrix (cf. the left singular vectors of the matrix SVD), time coefficients factor matrix (cf. the right singular vectors of the matrix SVD), and parameter coefficients factor matrices. Now a reduced basis for an unsampled parameter value can be computed by interpolating the relevant rows of parameter coefficients factor matrices and recombining them with the core tensor. We show that in terms of the resulting reduced basis this is equivalent to computing the SVD of appropriately interpolated state trajectory snapshots. However, due to the MLSVD decomposition step and the consequent data compression, TPOD is more time and memory efficient.

To demonstrate the performance of TPOD, we apply it to community benchmarks with one and two parameters and discuss its approximation quality as well as its runtime and memory consumption.

Model hierarchy of upper-convected Maxwell models with regard to simulations of melt-blowing processes

Manuel Wieland (*Fraunhofer ITWM, Germany, Universität Trier, Germany*)

09:50

Walter Arne (*Fraunhofer ITWM, Germany*)

Nicole Marheineke (*Universität Trier, Germany*)

Raimund Wegener (*Fraunhofer ITWM, Germany*)

In melt-blowing processes polymeric fiber jets are extruded into turbulent high-speed airflow leading to a significant thinning of the fiber diameters down to micro- and nano-scale. String models supplemented with viscoelastic material laws build a suitable basis for the modeling and simulation of fibrous jets in such production processes. We present a model hierarchy of upper-convected Maxwell models, whereby the initial model originates asymptotically from a

three-dimensional instationary boundary value problem. For the efficient simulation of industrial melt-blowing setups with incorporation of turbulent fluctuations the turbulent effects from an underlying k- ϵ description of the airflow are reconstructed and coupled into the fiber models. Within the model hierarchy, the simulation results are analyzed and evaluated with respect to efficiency and accuracy.

Efficient structural reliability analysis coupling an adaptive subset simulation and PGD model reduction

Annika Robens-Radermacher (*Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*)

10:10

Jörg Unger (*Bundesanstalt für Materialforschung und -prüfung (BAM), Germany*)

The key point of structural reliability analysis is the estimation of the failure probability. This probability is defined as the integral over the failure domain which is given by a limit state function. Usually, this function is only implicitly given by an underlying finite element simulation of the structure. It is generally not possible to solve the probability integral analytically. Therefore, simulation-based methods as well as methods based on surrogate modeling (or response surface methods) has been developed. Nevertheless, these variance reducing methods still require a few thousand calculations of the underlying finite element model, making reliability analysis computationally expensive for relevant applications.

The aim of this contribution is to increase the efficiency of structural reliability analysis by using the advantages of model reduction techniques. Model reduction is a popular concept to decrease the computational effort of complex numerical simulations while maintaining their accuracy. Coupling a reduced model with an efficient variance reducing sampling algorithm can reduce the computational cost of reliability analysis drastically.

In the developed method, a modification of the adaptive subset simulation based on Papaioannou et al. 2015 is used and coupled with a limit state function based on Proper Generalized Decomposition (PGD) (Chinesta et al. 2011). In the subset simulation the failure probability is expressed as a product of larger conditional failure probabilities. The intermediate failure events are chosen as a decreasing sequence. Instead of solving each conditional probability with a Markov-Chain approach, an importance sampling is used. It will be shown that the accuracy of the estimation depends then mainly on the number of samples for the last subproblem. On the other hand, the PGD approach is used to solve the structural problem a priori for a given parameter space (physical space plus all random parameters). The PGD approach results in an abacus, with which all solutions of a system depending on many parameters are simultaneously given. The approximation of the solution by a separated form allows a very efficient evaluation of the limit state function in the sampling algorithm. In the talk, the coupled PGD - adaptive subset simulation method is used to estimate the failure probability of examples with different complexity. The convergence, the error propagation as well as the saving in computational time will be discussed.

Chinesta et al., Arch. Comput. Meth. Eng. 18(4), 2011

Papaioannou et al., Prob. Eng. Mech. 41, 2015

S22.02 | Scientific computing

Date: February 19, 2019

16:30-18:30

Room: HS 42

IMEX-ODTLES: A multi-scale and stochastic approach for highly turbulent flows

Juan Medina (*BTU Cottbus-Senftenberg, Germany*)

16:30

Christoph Glawe (*Robert Bosch GmbH, Germany*)

Tommy Starick (*BTU Cottbus-Senftenberg, Germany*)

Mark Simon Schöps (*BTU Cottbus-Senftenberg, Germany*)

Heiko Schmidt (*BTU Cottbus-Senftenberg, Germany*)

The stochastic One-Dimensional Turbulence (ODT) model is used in this work in combination with a Large Eddy Simulation (LES) approach, in order to illustrate its potential for highly turbulent flows, which are in general not accessible for classical Direct Numerical Simulations (DNS) of the three-dimensional Navier-Stokes equations.

Although the idea of using ODT as a subgrid model for LES dates back to [1], the mathematical formalism and consistency of the model was not fully proved until Glawe formally contextualized it within the LES framework in [2]. The model was recently improved in terms of stability (see [3]) with an Implicit-Explicit (IMEX) numerical scheme based on the work of [4].

We use a new C++ implementation of the ODTLES code in order to analyze the performance of the model in a classical incompressible turbulent channel flow problem. The numerical logic of the model is analyzed in order to propose a modest parallelization approach, which aims to maximise the Monte Carlo ensemble calculation features of the standalone application of ODT. Some subtle variations in the interpretation of the IMEX scheme proposed in [3] are also analyzed in order to measure their impact on the performance of the code.

The parallel efficiency in terms of time-per-step against number of cores is evaluated, as well as the numerical results for the mean and RMS velocity profiles obtained with the different variations of the IMEX scheme. All ODTLES numerical results concerning velocity dynamics are compared against DNS data from [5].

References

- [1] R. C. Schmidt, A. Kerstein, S. Wunsch, V. Nilsen, Near-wall LES closure based on One-Dimensional Turbulence modeling, *J. Comput. Phys.* 186 (2003) 317-355.
- [2] C. Glawe, ODTLES: Turbulence Modeling Using a One-Dimensional Turbulence Closed Extended Large Eddy Simulation Approach, PhD Thesis, Freie Universität Berlin (2015).
- [3] C. Glawe, J. Medina, H. Schmidt, IMEX based multi-scale time advancement in ODTLES, *Z. Angew. Math. Mech.* (2018) 1-17, <https://doi.org/10.1002/zamm.201800098>.
- [4] D. Cavaglieri, T. Bewley, Low-storage implicit/explicit Runge-Kutta schemes for the simulation of stiff high-dimensional ODE systems, *J. Comput. Phys.* 286 (2015) 172-193.
- [5] R. D. Moser, J. Kim, N. N. Mansour, DNS of Turbulent Channel Flow up to $Re_\tau = 590$, *Phys. Fluids* 11 (1998) 943-945.

Shape optimization with a one-way coupled Eulerian model for laminar particulate flow problems

Raphael Hohmann (*Fraunhofer ITWM, Germany, University of Kassel, Germany*)

16:50

Christian Leithäuser (*Fraunhofer ITWM, Germany*)

Andreas Meister (*University of Kassel, Germany*)

Wall impingement of small solid particles transported in a fluid can lead to unwanted erosion or accretion in bended pipes and bifurcations. In order to increase the durability of the duct for a given stationary laminar flow configuration we want to reduce these particle-wall collisions by optimizing the shape of the duct. For a sufficiently small volume percentage of the solid phase a one-way coupled approach is justified, where the carrier fluid can be treated independently of the particles, whose motion is mainly affected by drag, gravity and buoyancy. Using a fully Eulerian model in the limit of low particulate load we derive the adjoint equations and shape derivative for a cost function based on the momentum transfer of monodispersed particles onto the duct and present first numerical results.

Pressure Poisson equation for the stokes system

Douglas Ramalho Queiroz Pacheco (*Technische Universität Graz, Austria*)

17:10

Olaf Steinbach (*Technische Universität Graz, Austria*)

For the standard variational formulation of the Stokes system, we consider the pressure Poisson equation by choosing gradient fields as appropriate test functions. This results in an ultra-weak variational problem to find the pressure in L^2 , which allows the use of a piecewise constant approximation for the pressure. In this case, the test functions have to be of second order to guarantee conformity and stability. We will discuss the stability and error analysis and we provide some numerical experiments. Moreover, we will discuss some further applications of this approach which can be used for a stabilization of lowest order finite element approximations for the Stokes system, the elimination of the pressure to obtain a velocity based formulation without constraints, the analysis and simulation of Stokes eigenvalue problems, and the extension to space-time methods for Stokes, and Navier-Stokes.

Algorithmic differentiation of an industrial airfoil design tool coupled with the adjoint CFD method

Mladen Banovic (*Paderborn University, Germany*)

17:30

Ilias Vasilopoulos (*Rolls-Royce Deutschland*)

Andrea Walther (*Paderborn University, Germany*)

Marcus Meyer (*Rolls-Royce Deutschland*)

Computer Aided Design (CAD) systems and tools are considered essential for industrial design. They create and manipulate the geometry of a certain component with an arbitrary set of design parameters. However, it is a challenging task to incorporate the parametric description in a gradient-based shape optimization loop, since the CAD systems usually don't provide surface derivatives w.r.t. the design parameters of the model. The common process is to compute these derivatives with inaccurate finite differences. On the contrary, to get the exact derivatives, algorithmic differentiation (AD) can be applied if the CAD sources are available. In this study, the Rolls-Royce in-house airfoil design and blade generation tool Parablading is differentiated in forward mode of AD using the AD software tools ADOL-C and Tapenade. The Parablading tool is written both in C++ and Fortran, and therefore comes the necessity for mixed-language AD. ADOL-C is based on the operator-overloading concept and has been used to differentiate a large part of the sources written in C++. Tapenade is based on the source-transformation concept and has been used to differentiate the rest of the sources written in Fortran. Therefore, different parts of the differentiated Parablading sources are linked to correctly propagate the derivative information. Finally, the differentiated Parablading tool has been coupled with a discrete adjoint CFD solver that is part of the Rolls-Royce in-house HYDRA suite of codes, also produced by algorithmic differentiation. This differentiated design chain is used to perform gradient-based optimization of the TU Berlin TurboLab stator test-case w.r.t. minimize the total pressure loss and exit angle deviation objectives.

Accurate gradient computations for shape optimization via discrete adjoints in CFD-related multiphysics problems

Ole Burghardt (*TU Kaiserslautern, Germany*)
Nicolas R. Gauger (*TU Kaiserslautern, Germany*)

17:50

As more and more multiphysics effects are entering the field of CFD simulations, this raises the question how they can be accurately captured in gradient computations for shape optimization. The latter has been successfully enriched over the last years by the use of adjoints. One can think of them as Lagrange multipliers to the flow field problem linked to an objective function that depends on quantities like pressure or momentums.

Two quite different research fields have emerged to compute the adjoint vector field. Whereas in the first one it appears as the solution to a partial differential equation that is to be set up and subsequently discretized and solved (continuous approach), the other approach directly solves for it within the discretised formulation (discrete approach).

While the discrete adjoint method has shown significant advantages in terms of stability and accuracy, it should be emphasized that the replacement itself of the adjoint PDE model (which has to be determined in the first place) by techniques like automatic differentiation (AD) creates the opportunity for a very generic implementation which can be particularly exploited when it comes to multiphysics problems and gradient computations therein.

We will show in this talk how this can be done in an effective way that is also easily extendable for all kinds of other couplings. As the open-source CFD solver SU2 already provides a large functionality for AD together with a discrete adjoint solver for its flow solvers like for Navier-Stokes or RANS, it was chosen by us to develop a solver for coupled discrete adjoints.

We suppose that a valuable first application are so-called conjugate heat transfer problems which are gaining more and more interest from the automobile and aeronautics industry. Typically, they consist of fluid and solid domains where one cannot neglect the conservation of energy across their interfaces or where it is impossible to determine a temperature distribution in advance. Think, for example, of cooling devices or turbine blades in a high-temperature airflow.

We therefore present an implementation for this capability in SU2 as well and will demonstrate that the all adjoint fields and derived gradients are accurate by validating them for a generic test case against finite differences.

S22.03 | Scientific computing

Date: February 20, 2019
Room: HS 42

08:30-09:30

Dynamic selection limiter schemes for high density gradient simulations of supersonic rarefied gas flows

Rodion Groll (*Universität Bremen, Germany*)

08:30

In classical DSMC simulations the number of locally computed collisions can span over three orders of magnitude between the inflow and the outflow region of a De Laval nozzle shaped propulsion system. The quality of thrust results and the precision of the predicted angular exit velocity distribution is mainly influenced by collisions in the hyper-sonic exit region of the nozzle's diffuser. The imbalance between the need for precise flow prediction and the high numerical costs of a kinetic simulation of the high density portion of a nozzle flow leads to the usage of collision-selection limiter schemes. Static collision limiter schemes do not differentiate between regions with varying degrees of flow rarefaction and different DSMC particle densities. As a

result a decrease of prediction quality may be enforced in all flow regions of a DSMC simulation. Dynamic collision limiter schemes satisfy the need for consideration of different degrees of flow rarefaction and particle densities characteristic for nozzle flows in space propulsion systems. Hence the quality of predicted flow properties is improved by continuously adaptation of computed collisions on the local flow.

In the present publication characteristics and advantages of static and dynamic collision selection limiter schemes are discussed and compared. Influences of the schemes on the reduction of numerical cost and simulation time are presented. Discussion of results is carried out on basis of the discrete influence of multi-level grid coarsening and different elongations of the numerical time step on the quality of predicted flow quantities, using collision limiter schemes. Based on these results advantages and limits of the present models are opposed. The results presented show the advantages of a dynamic collision limitation on the high density inflow region of the nozzle flow, without distinctly decreasing the quality of numerical results.

Modeling and simulation of the aqueous humor flow in the anterior chamber

Vladislav Olkhovskiy (*University of Heidelberg, Germany*)

08:50

Elfriede Friedmann (*University of Heidelberg, Germany*)

One of the most common reason for blindness is glaucoma. The primary risk factor for the development of the vision loss in glaucoma is an increased intraocular pressure (IOP) and lowering the IOP is currently the only therapeutic option with proven efficiency. To understand the behaviour of the aqueous humor flow and of the IOP in the anterior chamber of the human eye, a mathematical model is developed. This model is given by Stokes and Darcy equations. With the help of the Darcy equation the mean pressure value in the Darcy domain is computed. This mean pressure value is incorporated into the Neumann boundary condition of the Stokes equation. The Stokes equation describes the aqueous humor flow in the anterior chamber and the Darcy equation describes the pressure in the trabecular meshwork which is a porous medium. The characteristic physical properties are given by the inflow rate of the aqueous humor at the ciliary body, the pressure of the episcleral veins and it is assumed that the cornea, the lens, the iris and the zornules are impermeable. Geometries for healthy eyes are considered. Numerical simulations using the Finite Element Method are performed in three dimensions. In the computation, mixed finite elements are used and the solution is generated with deal.ii software. The simulations cover the impact of specific changes of certain model parameters on the change of the IOP. Moreover, medical applications are discussed.

An accelerated boundary-domain integral method for three-dimensional fluid flow analysis

Jan Tibaut (*University of Maribor, Slovenia*)

09:10

Jure Ravnik (*University of Maribor, Slovenia*)

The rapid growth of computer power enables performing of more and more complex numerical simulations. However, the need to develop efficient numerical algorithms is always present. In this study, we propose an acceleration of an algorithm to solve the nonlinear system of Navier-Stokes equations. We present an accelerated Boundary domain integral algorithm (BDIM). The BDIM is a boundary element method based method, thus its computational demands scale as $O(N^2)$, where N is the number of grid nodes. This is due to the fact that the discretization procedure leads to fully populated matrices. By transforming the fully populated matrices into matrix parts with the H-matrix structure procedure and by applying approximation techniques, we can reduce the computational complexity of the method. Several approximation techniques exist, such as multipole approximation methods FMM (Fast multiple method), SVD (singular value decomposition method), Wavelet transform method or a Cross approximation method [1].

In this study, we solve the velocity-vorticity formulation of the Navier-Stokes equations and develop an accelerated algorithm for determination of the boundary vorticity in 3D based on the cross approximation method. We employ the modified Helmholtz fundamental solution as well as the Laplace fundamental solution to develop the algorithm. We test the developed algorithm using standard benchmark test cases for fluid flow and for coupled fluid flow and heat transfer. When using acceleration, we observe nearly linear $O(N \log N)$ scale up of computational demands. The results show that the increasing acceleration (matrix compression rate) has a negative influence on the solution accuracy. On the other hand, the solution accuracy increases with computational mesh density. We introduce the concept of optimal compression, which is based on the fact that the acceleration of the method should introduce an error of the same order of magnitude as the other sources of error in the numerical algorithm.

[1] J. Tibaut, L. Škerget, and J. Ravnik, ‘Acceleration of a BEM based solution of the velocity-vorticity formulation of the Navier-Stokes equations by the cross approximation method’, *Eng. Anal. Bound. Elem.*, vol. 82, no. C, pp. 17-26, 2017.

S22.04 | Scientific computing

Date: February 20, 2019
Room: HS 42

14:00-16:00

Mean-field surrogate models of (semi-)dilute particle suspensions

Alexander Vibe (*Universität Trier, Germany*)

14:00

Nicole Marheineke (*Universität Trier, Germany*)

We apply asymptotic expansions to deduce a mean-field approximation of a coupled particle-fluid system. The three-dimensional multi-scale problem consists of Navier-Stokes equations for the fluid flow coupled via Newton’s third law to a large number of small inertial particles of general shape. Since a resolution of the particle boundaries in numerical simulations is not feasible due to the particle number as well as their size, surrogate models are desirable which approximate the original system. The particles are assumed to be small and to maintain a minimal distance between each other, while their density is scaled such that different asymptotic inertia regimes may be defined. By using appropriate constraints on particle number and distance, the particle dynamics simplify to a coupled nonlinear ODE system of interacting particles via hydrodynamic forces. It amounts to the definition of a convection of particle position and orientation by the underlying carrier fluid, which is in turn coupled to particle induced forces in the bounded system domain. The resulting system of equations treats the suspension as a homogeneous fluid and describes its momentum by a Navier-Stokes like equation coupled to a transport equation for the probability density function of the particle orientation and position. The particle inertia, number and minimal distance lead to different effects in the resulting system.

Simulation of generalized Newtonian fluids with the smoothed particle hydrodynamics method

Milos Simeunovic (*University of Stuttgart, Germany*)

14:20

Holger Steeb (*University of Stuttgart, Germany*)

This work proposes a computational method for modeling and solving three dimensional single phase flow of a generalized non-Newtonian fluids. Due to the versatility of industrial and technical applications, it is important to understand and predict the specific rheological behavior that occurs in non-Newtonian flow. For the reason of large deformations and presence of free surface flow, we use the Lagrangian Smoothed Particle Hydrodynamics (SPH) as a simulation

technique. The non-Newtonian solver is implemented into the general purpose particle framework HOOMD-blue [1,2], which allows for massive parallel CPU and GPU simulations. We extensively tested the numerical accuracy of the model by investigating confined Poiseuille flow between parallel plates. Furthermore, we investigated the evolution of free surface which is compared to the experimental result of the broken dam problem [3]. As an application example we have done the slump test simulation that is often used in practice to examine concrete workability. Moreover, we have observed in further detail the cone diameter, height, flow time, the final shape and the influence of the rheological model parameters as well as the boundary conditions related to the final cone configuration.

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Parallel FE solver for the stationary Navier-Stokes equations with adaptive grid refinement using a PU dual-weighted residual method

Jan Philipp Thiele (*Leibniz University Hannover, Germany*)

14:40

Thomas Wick (*Leibniz University Hannover, Germany*)

In this presentation, we combine parallel computing and mesh adaptivity for the Navier-Stokes equations, which is an ongoing trend in Computational Fluid Dynamics. A common problem arises in the evaluation of specific goal functionals. These functionals could be technical quantities like drag or lift coefficients as well as point-values or (local) averages. The Dual Weighted Residual Method (DWR) proposed in [3] is successful in solving these problems and has been used in many different CFD applications e.g. [1],[2]. In [4] a different approach to error localization using a partition of unity (PU) for the DWR method was proposed. This technique is now applied to the simulation of stationary Navier-Stokes flow. Since practical problems - specifically in 3D - require a considerable amount of degrees of freedom, a focus in this talk lies in the parallel solution. To substantiate the method the 2D-1 (steady) test case as described in [5] is computed. This test allows for the scalability analysis of the parallel computations.

[1] Braack, Richter: Solutions of 3D Navier-Stokes benchmark problems with adaptive finite elements

[2] Besier, Rannacher: Goal-oriented space-time adaptivity in the finite element Galerkin method for the computation of nonstationary incompressible flow

[3] Becker, Rannacher: Weighted a posteriori error control in FE methods

[4] Richter, Wick: Variational localizations of the dual weighted residual estimator

[5] Schaefer, Turek: Benchmark Computations of Laminar Flow Around a Cylinder

Simulation of calcium waves in a heart cell on modern multi-core parallel computing platforms

Carlos Barajas (*University of Maryland, Baltimore County, United States of America*) 15:00
Stefan Kopecz (*University of Kassel, Germany*)
Andreas Meister (*University of Kassel, Germany*)
Bradford E. Peercy (*University of Maryland, Baltimore County, United States of America*)
Matthias K. Gobbert (*University of Maryland, Baltimore County, United States of America*)

The flow of calcium ions in a heart cell is modeled by a system of time-dependent reaction-diffusion equations. The highly non-smooth nature of the source terms, the large number of calcium release sites requiring high-resolution meshes, and the need for long-time simulations up to large final times are among the challenges for convergent and efficient numerical methods for this problem. State-of-the-art distributed-memory computer clusters contain multi-core CPUs with 36 or more cores. We demonstrate the power of such clusters for long-term simulations for this application problem and study the strong and weak scalability of hybrid MPI+OpenMP code.

Analysis of acoustic wave propagation in composite laminates via a spectral element method

Elias Perras (*University of Siegen, Germany*) 15:20
Chuanzeng Zhang (*University of Siegen, Germany*)

The analysis of the acoustic or elastic wave propagation phenomena in the time-domain is computationally expensive. An often-cited rule of thumb is to use at least ten nodes per wavelength if using quadratic shape functions, and even more nodes are necessary in order to achieve highly accurate numerical results. For large-scale domains, this results in a large linear system of algebraic equations, which must be solved for several thousands of time-steps and hence requires a vast amount of the computing time.

In this paper, a spectral element method (SEM), which is a variant of the finite element method (FEM) by using high-order shape functions with non-equidistant node distributions, is presented in order to investigate the acoustic wave propagation problems taking the fluid-structure interaction into account with a minimum of required degrees of freedoms (DOFs). Hence, the computing time for solving the linear system of linear algebraic equations is reduced while maintaining a high accuracy. The element matrices are computed using the Lobatto-quadrature method, which results in a diagonal element mass matrix. For fluid-structure interaction problems in acoustics, a non-symmetric sparse mass matrix is obtained. If using an explicit time-integration scheme only the mass matrix becomes the coefficient matrix of the linear system, and due to its high sparsity the solution process is very efficient.

In this work, the SEM is implemented and applied for the analysis of the transient behavior of the laminated composite structures excited by acoustic waves. Numerical examples will be presented and discussed to show the efficiency of the SEM in the time-domain compared with the standard FEM for applications in acoustics considering the fluid-structure interaction.

Parallel-in-time solution of eddy current problems

Stephanie Friedhoff (*Bergische Universität Wuppertal, Germany*)

15:40

Jens Hahne (*Bergische Universität Wuppertal, Germany*)

Sebastian Schöps (*Technische Universität Darmstadt, Germany*)

Maxwell's equations are an essential tool in the numerical simulation of problems in electrical engineering. A standard approach for the simulation of electrical machines is to neglect the displacement current in Maxwell's equations, yielding the so-called magnetoquasistatic approximation or, synonymously, the eddy current problem. Typically, solution algorithms for the time-dependent eddy current problem are based on a time-marching approach, solving sequentially for one time step after the other. The computational complexity of such approaches is high, particularly if long time periods have to be considered as, for example, in the case of simulating the start-up of an electrical machine. One approach for reducing the simulation time is with parallel-in-time integration techniques.

In this talk, we consider the usage of parallel-in-time algorithms of the Parareal [1] and multigrid-reduction-in-time (MGRIT) [2] methodologies for the parallel-in-time solution of the eddy current problem. We show that for a two-dimensional model problem for a coaxial cable model, a significant speedup can be achieved in comparison to sequential time stepping. Eventually, Parareal and MGRIT will be applied in the numerical optimization of electrical machines within the industrial-driven research project PASIROM, funded by the German Federal Ministry of Education and Research.

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S22.05 | Scientific computing

Date: February 20, 2019

16:30-18:30

Room: HS 42

Computational aspects of a bound of Lagrange

Doru Stefanescu (*University of Bucharest, Romania*)

16:30

We consider the bound $R + \rho$ of Lagrange and we obtain some improvements of it. We also discuss the efficiency of this bound of Lagrange and of its refinements.

J.-L. Lagrange, in his *Traite de la resolution des equations numeriques*, Paris (1798), has given two bounds for the largest positive root of a univariate polynomial with real coefficients. His second bound, called $R + \rho$, was reconsidered recently in publications on the numerical computation of polynomial roots and related results were implemented for efficient computations. We present some new results on this bound of Lagrange. For example, we prove that an upper bound for the roots of a particular cubic equation is an upper bound for the absolute values of the roots of a given polynomial.

We obtain estimates for the largest positive root of the particular associated polynomial H and we obtain further refinements. There are given comparisons among bounds for positive roots and we analyze the quality of the estimates. There are given estimates for the costs and there are given evaluations with respect to the threefold of polynomials.

A performance comparison of different shell elements for upper bound limit analysis

Vitezslav Stembera (*TU Wien, Austria*)

16:50

Josef Füssl (*TU Wien, Austria*)

The prediction of the collapse load (limit load) of a structure made of a material exhibiting elastic plastic behavior is very often of practical interest. The standard approach to obtain such collapse loads is based on iterative calculation schemes using classical nonlinear finite element methods, as, e.g., can be found [1].

However, as an alternative approach the so-called finite-element-based limit analysis (FELA) can be applied. This approach is based on limit theorems, first formulated by A.A.Gvozdev in 1938. Thereby, the collapse load is obtained as the minimum of a certain optimization problem, either considering kinematically compatible velocity fields (upper bound approach) or statically admissible stress fields (lower bound approach) within the structure, at the time instant of collapse. Thus, the whole load history doesn't need to be taken into account, resulting in a much more stable and efficient approach compared to the standard scheme based on classical finite element formulations. The two significant disadvantages of the FELA method, which are the assumption of geometrical linearity and ideal plasticity, can be overcome by the so-called sequential finite element limit analysis (SFELA), as, e.g., shown in [2]. Thereby, the FELA method is called repeatedly, where the geometry and the plastic strain is updated after each iteration.

In this work, one new and several well-known finite elements from classical FE formulations are implemented into an upper bound approach for shell structures. To the material a von Mises type strength criterion for shell elements (Ilyushin criterion) is assigned and isotropic hardening is considered. By means of different benchmark examples, the performance of these new elements is evaluated and the effect of different adaptive meshing strategies is investigated. Finally, it is shown that shell elements with improved drilling rotations interpolation are able to significantly increase the efficiency of SFELA calculations compared to existing shell element formulations. Moreover, the best possible combination of shell element and adaptive meshing strategy is highlighted and discussed.

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Partitioned adaptive multirate time integration for coupled systems of ODEs

Philipp Birken (*Lund University, Sweden*)

17:10

Peter Meisrimel (*Lund University, Sweden*)

We consider time integration methods for more complex coupled-systems. As a basic paradigm we consider partitioned methods, meaning that we aim to reuse existing software components. Furthermore, we want a solver that can adaptively work on multiple timescales, uses higher order methods in time and can solve subproblems in parallel, while performing load-balancing to maximize resource use. While there are methods and software to solve coupled problems, these feature only a subset of the desired properties.

Here, we employ a novel waveform-iteration approach using continuous data exchange. With a waveform iteration method, a process uses prescribed data at the interface over a time window and will provide the same to the other processes. In the classical methods, this data exchange is

done at the end of each time window and the methods are either slow in convergence (Jacobi) or not parallel (Gauß-Seidel). To get the best of both, we solve in parallel, exchange all new data and use it if possible. This way we get the parallelism from a Jacobi approach and improved convergence by directly employing new data.

Current results show the potential in terms of efficiency and most of the other desired properties are inherent to waveform-iteration type methods.

Simulating coupled free and porous media flow with lattice Boltzmann methods

Christoph Schwarzmeier (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*) 17:30

Ulrich Rüde (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

The lattice Boltzmann method is an efficient and highly parallelizable approach for solving the incompressible Navier-Stokes equations. It is well suited for the simulation of complex systems, such as fluid flow through porous media. Based on geometrically fully resolved 2D and 3D test scenarios, we investigate the interaction of free and porous media flow using large scale lattice Boltzmann simulations. The results provide first-principle insights into the physical processes in the porous medium and the flow behavior at the interface region.

A modified lattice Boltzmann formulation with adaptive numerical dissipation through independent control over higher-order moments

Seyed Ali Hosseini (*University of Magdeburg "Otto von Guericke", Germany, Université Paris-Saclay, France, International Max Planck Research School (IMPRS) for Advanced Methods in Process and Systems Engineering, Germany*) 17:50

Nasser Darabiha (*Université Paris-Saclay, France*)

Dominique Thévenin (*University of Magdeburg "Otto von Guericke", Germany*)

The lattice Boltzmann method, thanks to the highly local nature of its discrete time-evolution operators, has become a popular tool for computational fluid dynamics over the past couple of decades, and has in parallel been extended to a plethora of areas such as multi-species and multi-phase flows. However, this rather popular numerical tool performs poorly in under-resolved high Reynolds number simulations. This is partly caused by -just like other finite-differences solvers- inconsistent dispersion-dissipation behavior of the scheme at higher wavelengths. In classical solvers higher-order filters are usually introduced in order to maintain the order of accuracy of the scheme while dissipating Gibbs oscillations emanating from this inconsistency at high wavelengths. In the context of the lattice Boltzmann method, the "diffusion" coefficient controlling higher-order error terms can be decoupled from the physical dissipation coefficient (i.e., viscosity) using the lattice Kinetic formulation. This formulation comes with an additional free parameter controlling higher-order moments appearing in the asymptotic analysis of the scheme. To establish an efficient balance between numerical higher-order dissipation and dispersion, the free parameter must be tied to a flow state indicator. One of the simplest indicators, used in the context of the lattice Boltzmann method, and also shown to be closely tied to numerical instability, is the positivity of the particle distribution function.

In the present work, the concept of positivity of the distribution function along with the lattice kinetic scheme are used to perform stable under-resolved simulations. The performances of this approach are tested through a comparative study of the classical 3-D Taylor-Green vortex using a wide range of resolutions.

Discontinuous Galerkin methods with new multigrid preconditioners

Lea Miko Versbach (*Lund University, Sweden*)

18:10

Philipp Birken (*Lund University, Sweden*)

Gregor Gassner (*University of Cologne, Germany*)

We consider compressible turbulent flow problems which arise for example in the design of next generation jet engines, air frames, wind turbines or star formation. These can have a 100 million unknowns, thus a fast parallel solver with low memory footprint is needed. A suitable high order method for solving these problems are implicit Discontinuous Galerkin (DG) methods. In this talk we study the DG spectral element method with Gauss-Lobatto-Legendre nodes (DGSEM-GL) for nonlinear conservation laws. It has been proven that DGSEM-GL can be written as a specific finite volume (FV) method, see Fischer et al. (2013) and Gassner (2012). This allows to apply known theory from FV methods to the DGSEM-GL formulation.

Our main interest are multigrid (MG) methods. These are iterative methods designed to solve equation systems associated with discretized differential equations and are tailored to the problem to be extremely efficient. Moreover, they can be used to construct preconditioners for Newton-Krylov schemes.

An implicit DGSEM discretization results in a nonlinear system which has to be solved. By constructing a good preconditioner we can improve the convergence rate of the Newton-Krylov scheme to get a fast and efficient solver. MG methods for FV discretizations have a long history, thus we construct MG methods for approximations to the equivalent FV discretization. In the construction of MG methods, the smoother plays an important role. We consider optimized Runge-Kutta smoothers from Birken (2012) and W-smoothers from Birken (2018) and examine their influence on the quality of the resulting preconditioner. We gain an improved convergence rate using FV based MG preconditioners for DGSEM as described above. The choice of smoother in the MG preconditioner is visible in the convergence rate and using W smoothers gives the best convergence rate for our numerical tests. We will show one-dimensional numerical results.

S22.06 | Scientific computing

Date: February 21, 2019

08:30-10:30

Room: HS 42

On empirical system Gramians

Sara Grundel (*MPI Magdeburg, Germany*)

08:30

Christian Himpe (*MPI Magdeburg, Germany*)

Jens Saak (*MPI Magdeburg, Germany*)

State-space realizations of input-output systems or control systems are a widely used class of models in engineering, physics, chemistry and biology. For the qualitative and quantitative classification of such models, the system-theoretic properties of controllability and observability are essential, which are encoded in so-called system Gramian matrices. For linear systems these Gramians are computed as solutions to matrix equations; for nonlinear or parametric systems the data-driven empirical system Gramians approximate the actual system Gramians. These empirical Gramians have manifold applications, for example in model reduction or decentralized control of nonlinear systems, as well as sensitivity analysis, parameter identification or combined state and parameter reduction of parametric systems. With a focus on model reduction, the various empirical-Gramian-based techniques are demonstrated on a nonlinear, hyperbolic, parametric input-output system, using the open-source empirical Gramian framework - emgr - for MATLAB and Octave.

Criss-cross algorithms for computing the spectral value set abscissa and radius

Peter Benner (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

08:50

Tim Mitchell (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

Consider a linear dynamical system defined by a single matrix. Often more relevant than the question of theoretical stability is how much uncertainty can be tolerated before stability is no longer guaranteed. This perspective leads to the concepts of pseudospectra and the distance to instability but, for systems with input and output, uncertainty is modeled by perturbations with known structure. Thus, structured analogues of pseudospectra and the distance to instability are also considered, respectively spectral value sets and the complex stability radius (perhaps better known by its reciprocal, the H-infinity norm). Computing the distance to instability was first addressed by Byers using a level-set method, which shortly thereafter, was extended to H-infinity norm computation. More recently, related "criss-cross" algorithms were proposed to compute the pseudospectral abscissa and radius. We extend and refine these ideas further to compute the spectral value set abscissa and radius, with efficiency and robustness improvements that are even relevant for the special case of pseudospectra. Implementations of our new algorithms are available in the MATLAB-compatible open-source software library ROSTAPACK: ROBust STABILITY PACKAge.

Accelerated computation of the matrix disc function via Direct Acyclic Graph Scheduling

Martin Köhler (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

09:10

Jens Saak (*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*)

The Matrix Disc Function is a tool for spectral analysis of generalized eigenvalue problems and for the solution of matrix equations, like the Discrete-time Algebraic Riccati Equation (DARE). The matrix disc function is normally computed using an iterative scheme, the so called "Inverse Free Iteration". This scheme mainly consists of a QR decomposition and the partial application of the Q factor in each iteration step. Practical results show that the QR decomposition, as implemented in standard software packages like LAPACK, does no longer scale well on modern multi- and many-core computers. This leads to a bad utilization of the CPUs compared to similar algorithms, like the Matrix Sign Function iteration, and slows down the overall computation. To overcome this scalability problem, we propose a specialized QR decomposition which extends the structure preserving approach of Marqués et. al. presented in 2007. We demonstrate how a directed acyclic graph scheduling, as it became available in OpenMP 4, can be used to introduce parallelism outside the involved BLAS and LAPACK subroutines. Regarding modern computer architectures (especially their memory hierarchy) we further optimize the data layout to increase the data locality. Experiments, for a random problem of dimension 20 000, show that our optimization reduces the time to compute one QR decomposition by 61.6% from 60.13s to 23.11s compared to QR decomposition from Intel's MKL library on a 32-core Intel Xeon Skylake system.

Adaptive space-time isogeometric analysis of parabolic initial-boundary value problems

Ulrich Langer (*Johannes Kepler University Linz, Austria*)

09:30

Svetlana Matculevich (*RICAM, Austria*)

Repin Repin (*University of Jyväskylä, Finland, St.Petersburg Department of Steklov Mathematical Institute RAS, Russia*)

In this paper, we generalize results obtained in our preceding papers to locally stabilized space-time isogeometric analysis (IgA) schemes for parabolic problems in fixed and moving spatial computational domains. In particular, we derive new a priori and a posteriori error estimates including estimates for low-regularity solutions. Low-regularity solutions can arise from initial- and boundary conditions, non-smooth parts of the boundary, jumping coefficients (different materials), and last but not least, non-smooth (distributional) right-hand sides.

The authors would like to thank the Austrian Science Fund (FWF) for the financial support of the NFN “Geometry + Simulation” under the project grant S 117-03.

An eigensolver for the Hermitian Dirac operator with multigrid acceleration

Artur Strebel (*University of Wuppertal, Germany*)

09:50

Andreas Frommer (*University of Wuppertal, Germany*)

Karsten Kahl (*University of Wuppertal, Germany*)

Matthias Rottmann (*University of Wuppertal, Germany*)

We introduce a Jacobi-Davidson type eigensolver which uses a multigrid preconditioned FG-MRES solver as inner method. This method is used in lattice QCD, where eigenvalues of the Hermitian Dirac operator are needed to accelerate otherwise too expensive stochastic approaches. The main focus is the synergy between the outer and the inner solver, as well as several other strategies to make our approach scalable with respect to the lattice size.

Afterwards we show how this eigensolver can in turn be incorporated into the multigrid method as a generalized setup procedure, improving convergence speed and overall runtime in certain scenarios.

S22.07 | Scientific computing

Date: February 21, 2019

14:00-16:00

Room: HS 42

Tensor decompositions and Monte Carlo: compete or combine?

Sergey Dolgov (*University of Bath, United Kingdom*)

14:00

Karim Anaya-Izquierdo (*University of Bath, United Kingdom*)

Colin Fox (*University of Otago, New Zealand*)

Robert Scheichl (*University of Heidelberg, Germany*)

Decomposition by tensor products is a potent idea for breaking the curse of dimensionality in the numerical treatment of multivariate functions. It has multiple manifestations nowadays, ranging from classical Fourier series and low-rank matrix factorizations to complex tensor network states in quantum physics. For many high-dimensional functions used for statistical purposes (such as probability density functions) there exists numerical and/or theoretical evidence that these functions admit accurate low-cost approximations by tensor (Cartesian) products of univariate

factors, provided that the variables are "weakly" coupled in some statistical sense. Numerical integration and other linear operations on such functions become very efficient, as they can be carried out on the low-dimensional factors instead.

On the other hand, Monte Carlo methods have become a state of the art in statistics because of their applicability to virtually any (e.g. discontinuous) functions. However, for smooth functions their algebraic convergence with the famous rate of $1/2$ is often seen as unappealing and contrasted to much faster (e.g. exponential) convergence of the Gaussian quadrature combined with tensor decompositions.

This talk will present a new idea of unifying the two approaches for mutual benefits. In principle, the Monte Carlo sampling is already used to bootstrap the construction of tensor product approximations in cross interpolation or tensor completion methods, since sampling is the only way we can interrogate a general function. However, this process can be reversed: a tensor approximation of a probability density function

allows to compute tailored Monte Carlo (or quasi Monte Carlo) points with a smaller variance by the Rosenblatt transformation. Alternatively, the Monte Carlo quadrature (after MCMC rejection or Importance Weighting) is able to clean up the tensor approximation error. We demonstrate that this hybrid approach can outperform Delayed Rejection MCMC in Bayesian inverse problems.

Application of modern tensor formats to quantum chemistry

Michael Götte (*TU Berlin, Germany*)

14:40

Reinhold Schneider (*TU Berlin, Germany*)

One part of Quantum Mechanics is electronic structure theory (EST). In EST one of the goals is to predict properties (e.g. the ground state energy) of atomic and molecular systems (A&MS). In physics, one way of tackling the high-dimensional Schrödinger equation arising in EST is through the Density Matrix Renormalization Group (DMRG) introduced in 1992. In the last 10 to 15 years it became apparent that the DMRG is equivalent to an ALS-like tensor method on a specific tensor tree network (TTN), i.e. the tensor train (TT) format. This opened the possibility to combine advances from chemistry and physics with the mathematical field of tensor product methods.

Recent research investigates different TTN formats to reduce the system sizes of the arising local (with respect to a tensor network node) sub-problems through proper identification of the entanglement in the A&MS. Entanglement is the key quantum mechanical resource to overcome the curse of dimensionality with low rank tensor optimization methods (TOM).

In this talk I will give a comparison analysis of the TT format with the hierarchical tucker (HT) format for EST for the calculation of the energy ground state of A&MS (like H₂O). This especially includes implementational details on the construction of the involved tensor operators in second quantization.

The calculations are performed in the novel C++ Tensor library Xerus (<https://libxerus.org/>), which is intended to be an easy to use, computational efficient implementation for TOMs developed by the group of Prof. Reinhold Schneider. A brief introduction to Xerus is also part of the talk.

Double-grid integration with interpolation-projection (DoGIP): an application to finite element method

Jaroslav Vondřejc (*Technische Universität Braunschweig, Germany*)

15:00

This contribution is focused on the double-grid integration with interpolation-projection (DoGIP), which is a novel discretisation approach of variational formulations. The method, introduced for Fourier-Galerkin method, is presented here as a more general method with an

application to the finite element method (FEM). The approach is based on treating the trial and a test functions in variational formulation together, which leads to the decomposition of a linear system into interpolation and (block) diagonal matrices. It usually leads to reduced memory demands, especially for higher-order basis functions, but with higher computational requirements. The numerical examples are studied here for two variational formulations: weighted projection and scalar elliptic problem modelling e.g. diffusion or stationary heat transfer. This paper also open a room for further investigations and applications, which will be discussed.

Reference:

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A matrix-free approach for finite-strain hyperelastic problems using geometric multigrid

Denis Davydov (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*) 15:20

Jean-Paul Pelteret (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

Daniel Arndt (*Heidelberg University, Germany*)

Paul Steinmann (*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*)

The performance of finite element solvers on modern computer architectures is typically memory bound. The main cause for this is that loading matrix elements from RAM into CPU cache is significantly slower than performing the arithmetic operations when solving the problem. In order to improve the performance of iterative solvers within the high-performance computing context, so-called matrix-free methods are widely adopted in the fluid mechanics community, where matrix-vector products are computed on-the-fly.

In this work, we extend the application of matrix-free approaches to problems in solid mechanics and investigate different implementations of the finite-strain hyperelastic tangent operator numerically. In order to improve the convergence behavior of iterative solvers, we also propose a method by which to construct level tangent operators and employ them to define a geometric multigrid preconditioner. Our implementation employs MPI and Intel Threading Building Blocks parallelization, and SIMD vectorization. The performance of the matrix-free operator and the geometric multigrid preconditioner is compared to the matrix-based implementation with an algebraic multigrid preconditioner for a representative numerical example of a heterogeneous hyperelastic material in two and three dimensions.

Optimal colorings of block smoothers in multigrid methods

Nils Kintscher (*University of Wuppertal, Germany*) 15:40

Karsten Kahl (*University of Wuppertal, Germany*)

Due to increasingly parallel computing environments block smoothers, i.e., domain decomposition methods, have become more and more important to achieve high efficiency in multigrid solvers as they can be easily parallelized and possess nice data locality. In order to realize the full potential of these block smoothers one has to color the blocks such that any two blocks of the same color decouple and thus can be processed in parallel. In this talk we show how to optimize the order in which colors should be processed using local Fourier analysis.

Local Fourier analysis (LFA) is a powerful tool used in the construction and analysis of multigrid methods. The fundamental idea of LFA is to leverage the connection between position space

and frequency space via the Fourier transform. That is, in case the involved operators can be described by stencils in position space, i.e., they possess a shift invariant structure, their Fourier transform yields so-called symbols, which can be handled much more easily.

LFA yields exact convergence rates for multigrid methods applied to problems with periodic boundary conditions and yields good estimates in case other boundary conditions are employed and appropriate additional processing is applied. Due to this fact, LFA is one of the main tools in the quantitative analysis of two- and multi-grid methods.

Using LFA we show that the ordering in which the colors are processed can have a large influence on the convergence rate of the resulting two-grid method by means of local Fourier analysis.

In order to be able to calculate the optimal color ordering we use symmetries of the underlying lattices which describe the shift-invariance of the smoothing iteration and the coarse-grid correction to reduce the factorial number of possible color permutations. Interestingly, we found that while the differences in convergence rates are rather small when only doing an analysis of the smoothing iterations, these can be substantial (an order of magnitude) when including the coarse-grid correction in the analysis.

S22.08 | Scientific computing

Date: February 22, 2019

08:30-10:30

Room: HS 42

Evaluating neural networks and quantum computing for solving mechanical problems

André Mielke (*University of Stuttgart, Germany*)

08:30

Tim Ricken (*University of Stuttgart, Germany*)

Artificial neural networks (ANNs) had a huge impact on our world in the last decade and still present us with growing opportunities for applications in a wide array of vastly different fields. While a lot of work is being done to incorporate advanced techniques into well-tested approaches to engineering problems [Belfiore and Rudas(2014)], cutting edge examples are rarely investigated from a performance to time investment ratio perspective. Here, we will present problems solved with classical as well as machine learning methods and compare invested time to runtime of the models.

In general, the defining ability of ANNs is the approximation of any given non-linear function to arbitrary precision, provided suitable activation functions are used [Cybenko(1989), Kreinovich(1991)]. This property can be exploited to reduce computation time for large models in multiple ways. It is possible to apply ANNs as a non-linear model order reduction technique or to express certain parts of the computation by trained ANNs. Additionally, replacing constitutive relations with data-driven approaches shows promising results [Conti et al.(2018)]. A further interesting developing field is quantum computing. Currently, the quantum algorithm zoo [Jordan(2018)] lists 59 algorithms of which a few can be applied to parts of mechanical calculations and even used on real hardware [IBM(2018)]. We evaluate the feasibility of using these algorithms to accelerate parts of common tasks in engineering problems and give an outlook on work that still needs to be done.

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Geometric a-priori evaluation of sampling designs

Rebecca Daum (*Technical University of Munich, Germany, Volkswagen AG, Germany*)

08:50

Many application questions in the automotive industry arise from highdimensional, complex settings and deal with strongly nonlinear behavior of objective criteria. Surrogate modeling based on suitable sampling designs is a cross-application technique that is widely used for virtual vehicle development. One kind of complexity results from the incidence of both categorical and continuous parameters and puts special demands on the sampling design. The Optimal Sliced Latin Hypercube Design (OSLHD) provides a solution: It makes use of the deterministic behavior of simulations and transfers the advantages of a purely continuous Latin Hypercube Design (LHD) to a mixed set of one categorical and several continuous parameters. For a given number of sample points (where sample points correspond to simulation runs), continuous parameters, and categorical parameter levels, the OSLHD constructs a space-filling sampling design.

However, standard techniques for sampling design assume linear or simple nonlinear relations. When applied on strongly nonlinear settings and without knowing the simulation results, we cannot evaluate beforehand if the number of sample points in an OSLHD is sufficiently large. If not, we cannot increase the number of sample points by simply adding further points while keeping the previous ones unchanged. Instead, it is necessary to construct a new sampling design. Since complex simulations for virtual vehicle development require a high computational capacity, the computational effort increases. We show that a geometric a-priori approach using Voronoi regions and Delaunay triangulations is suitable for identifying adjacency relations. This allows us to evaluate the sampling design for strongly nonlinear settings before conducting the simulations. We identify the adjacency relations of sample points on a restricted parameter space using their Delaunay triangulation, which we adjust by eliminating those edges related to sample points that only share a Voronoi edge outside the parameter space. This requires a detailed distinction of cases according to the positions of the Voronoi vertices. A difference-quotient-like ratio defined for two sample points serves as a quality criterion for the sampling design. Based on the adjacency relations, we estimate this ratio for neighboring sample points. Since strongly nonlinear behavior only occurs in small neighborhoods, this allows us to identify critical parameter areas and to refine the sampling design.

Our results show that the computational efficiency increases if we evaluate sampling designs before conducting complex simulations. This is an important advantage in virtual vehicle development. If limited computational capacity prevents a further refinement of the sampling design, we can evaluate the strength of identifiable nonlinear behavior. Since the OSLHD is independent of specific applications, we can apply the optimized sampling design to various same-sized questions. In conclusion, our results contribute to the efficient a-priori evaluation of sampling designs for strongly nonlinear settings and, therefore, to the increase of computational efficiency in virtual vehicle development.

Matrix-free multigrid solvers for phase-field fracture problems

Daniel Jodlbauer (*RICAM, Linz, Austria*)

09:10

Ulrich Langer (*RICAM, Linz, Austria*)

Thomas Wick (*IfAM, University Hannover, Germany*)

Fracture propagation problems are of high interest in different fields, ranging from material science to medical applications. To cope with the ever increasing demand to solve larger problems, efficient solvers need to be developed. In this talk we present a framework for the matrix-free solution to the phase-field fracture model with geometric multigrid methods. Using a standard matrix based approach for FEM requires lots of memory, which eventually becomes a serious bottleneck. A matrix-free approach avoids this and greatly reduces the amount of memory required, allowing to solve larger problems on standard hardware.

This work has been supported by the Austrian Science Fund (FWF) grant No. P-29181 ‘Goal-Oriented Error Control for Phase-Field Fracture Coupled to Multiphysics Problems’.

Adaptive concentric interpolation: a data-driven surrogate with application to nonlinear homogenization

Felix Fritzen (*Institute of Applied Mechanics, University of Stuttgart, Germany*)

09:30

The homogenization of nonlinear materials using interpolation techniques has seen come attention in the past years (e.g. [1, 2]) including applications to pseudo-plastic materials [2, 3]. A limitation of many existing approaches is the recourse to a prohibitively large number of required training computations which is needed due to the high dimension of the parameter space (six and higher). In [3] a dedicated sampling and interpolation strategy was proposed in order to reduce the amount of needed data: the RNEXP. Recently the generation of the sampling sites was refined and the interpolation method was generalized and renamed into Concentric Interpolation [4].

While CI is generally numerically efficient and accurate, the computational efficiency depends quadratically on the number of sampling directions. In the present study this quadratic dependency is relaxed by using adaptive refinement and anisotropic sampling. Thereby the overall computational efficiency can be increased considerably while the accuracy can be preserved or improved. Numerical results highlighting the improvements are presented.

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[2] J. Yvonnet, D. Gonazalez, Q.-C. He: Numerically explicit potentials for the homogenization of nonlinear elastic heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering* 198:2723-2737, 2009.

[3] F. Fritzen, O. Kunc: Homogenization of hyper-elastic solids using data-driven homogenization and reduced order modeling, *European Journal of Mechanics A/Solids* 69:201-220, 2018.

[4] O. Kunc, F. Fritzen: Generation of energy-minimizing point sets on spheres and their application in mesh-free interpolation and differentiation. *Advances in Computational Mathematics*, under review, 2018.

S23 | Applied operator theory

Organiser: Olaf Post (*Trier University, Germany*)
Jonathan Rohleder (*Stockholm University, Sweden*)

S23.01 | Applied operator theory

Date: February 19, 2019 08:30-10:30
Room: SR 06

Schrodinger operators exhibiting an abrupt change of the spectral character

Pavel Exner (*Czech Academy of Sciences, Czech Republic*) 08:30

In this talk we are going to discuss several classes of Schrödinger operators with potentials that are below unbounded but their negative part is localized in narrow channels. A prototype of such a behavior can be found in Smilansky-Solomyak model devised to illustrate that an irreversible behavior is possible even if the heat bath to which the systems is coupled has a finite number of degrees of freedom. We review its properties and analyze several modifications of this model, with regular or strongly singular potentials, or a magnetic field, as well as another system in which $x^p y^p$ potential is amended by a negative radially symmetric term. All of them have the common property that they exhibit an abrupt parameter-dependent spectral transition: if the coupling constant exceeds a critical value the spectrum changes from a below bounded, partly or fully discrete, to the continuous one covering the whole real axis. We also discuss resonance effects in such models. The results come from a common work with Diana Barseghyan, Andrii Khrabustovskyi, Jiří Lipovský, Vladimir Lotoreichik, and Miloš Tater.

Finite element solutions to a Sturm-Liouville transmission eigenproblem

Calin-Ioan Gheorghiu (*Romanian Academy, Romania*) 09:10
Bertin Zinsou (*University of the Witwatersrand, South Africa*)

An elliptic one-dimensional second order boundary value problem with transmission conditions is considered. The transmission conditions result from jumps in the coefficients of the equation. They require more complex analytical as well as numerical methods to solve the corresponding eigenvalue problem than in the case of continuous coefficients. We introduce a special Hilbert space along with an integral operator defined in it, in such a way that the problem under consideration can be interpreted as a spectral one for this operator. The eigenvalues, the eigenfunctions, as well as the integral solution of the problem are investigated. We show that eigenvalues are real and geometrically simple and the eigenvectors are orthogonal. Then the eigenpairs are computed numerically by a linear finite element method (FEM) applied to a variational (weak) formulation. This formulation includes the discontinuity of the derivative at the jump site. In order to solve the symmetric generalized eigenvalue problem (GEP) provided by FEM we have comparatively used the MATLAB built in functions `eig` and `eigs`, the latter with options to compute some of the largest or smallest in magnitude eigenvalues. It is well known that the second routine is applicable for sparse matrices as is the case with the matrices in the pencil of GEP. A convergence flag returned by `eigs` has been zero in all our numerical experiments, which means convergence. A positive lower bound for eigenvalues is provided. Neither for eigenvalues nor for eigenvectors could we find similar result in literature to compare with. In order to assess the numerical stability (accuracy) of eigenvalues computation with respect to the order of approximation as well as the physical (jump) parameter, we compute the so called relative drift of a particular

set of eigenvalues. Because we compute a large set of eigenvectors, actually their number equals the order of approximation, the accuracy in computing them is addressed by estimating their departure from orthogonality. The odd half of them are spurious (parasite) and are eliminated. They trivially satisfy the jump conditions. However, the eigenvectors become more oscillating as the mode order increases, after the eigenvalues have been sorted in increasing order. Extensive numerical results are displayed in order to confirm the analytical ones. Some open issues are mentioned.

The non-real spectrum of singular indefinite Sturm-Liouville operators with uniformly locally integrable potentials

Jussi Behrndt (*TU Graz, Austria*)

09:30

Philipp Schmitz (*TU Ilmenau, Germany*)

Carsten Trunk (*TU Ilmenau, Germany*)

In this talk we consider Sturm-Liouville differential operators related to the singular differential expression

$$\frac{1}{r} \left(- \frac{d}{dx} p \frac{d}{dx} + q \right)$$

on the real line, where the weigh r has indefinite sign, the potential q is uniformly locally integrable and $1/p \in L^\eta(\mathbb{R})$ for some $\eta \in [1, \infty]$. Explicit bounds on the non-real eigenvalues are introduced. These bounds depend basically on the number of sign changes of r and on norms of q and $1/p$.

Dirac systems on the semi-axis: reflection coefficients and Weyl functions

Alexander Sakhnovich (*University of Vienna, Austria*)

09:50

Dirac systems are of essential theoretical and applied interest. We discuss interrelations between the reflection coefficients and Weyl functions of Dirac systems and applications of these results. The talk is based on the paper [1] and some further developments. The research and talk are supported by the Austrian Science Fund (FWF) under Grant No. P29177.

References.

[1] A.L. Sakhnovich, Scattering for general-type Dirac systems on the semi-axis: reflection coefficients and Weyl functions, *J. Differential Equations* 265 (2018), no. 10, 4820-4834.

Self-adjoint Dirac operators on domains in \mathbb{R}^3

Markus Holzmann (*Graz University of Technology, Austria*)

10:10

Let $\Omega \subset \mathbb{R}^3$ be a bounded or unbounded domain with compact C^2 -smooth boundary. In this talk Dirac operators acting on functions which satisfy suitable boundary conditions that yield self-adjoint operators in $L^2(\Omega; \mathbb{C}^4)$ are discussed. Such operators are the relativistic counterparts of Laplacians on Ω with Robin-type boundary conditions. The self-adjointness of the operators is shown for a wide class of boundary values and the basic spectral properties are investigated. It turns out that there are some critical boundary values for which the spectral properties of the corresponding operators are of a completely different nature.

This talk is based on joint works with J. Behrndt and A. Mas.

S23.02 | Applied operator theory

Date: February 19, 2019

16:30-18:30

Room: SR 03

Everything is possible for the domain intersection of an operator and its adjoint

Christiane Tretter (*University of Bern, Switzerland*)

16:30

Yury Arlinskiiii (*East Ukrainian National University, Ukraine*)

In this talk it will be shown that even for very nice classes of linear operators such as maximal sectorial operators T everything is possible for the domain intersection $\text{dom } T \cap \text{dom } T^*$, even the most extreme case $\text{dom } T \cap \text{dom } T^* = \{0\}$.

Essential spectrum of operator pencils

Hannes Gernandt (*TU Ilmenau, Germany*)

16:50

In this talk, the essential spectra of linear operator pencils under perturbations are investigated. For this we associate linear subspaces, also called linear relations, with the operator pencil and use spectral perturbation theory for linear relations. In particular, we obtain sufficient conditions on the coefficients of the operator pencil that lead to invariance of the essential spectrum. Finally, the results are applied to an abstract differential-algebraic equation arising in the modelling of electric circuits. This talk is based on a joint work with N. Moalla, F. Philipp, W. Selmi and C. Trunk.

Friedrichs operators as dual pairs

Nenad Antić (*University of Zagreb, Croatia*)

17:10

Marko Erceg (*University of Zagreb, Croatia*)

Alessandro Michelangeli (*SISSA Trieste – International School for Advanced Studies, Italy*)

The Friedrichs (1958) theory of positive symmetric systems of first order partial differential equations encompasses many standard equations of mathematical physics, irrespective of their type. This theory was recast in an abstract Hilbert space setting by Ern, Guermond and Caplain (2007), and by Antić and Burazin (2010). In this work we make a further step, presenting a purely operator-theoretic description of abstract Friedrichs systems via the universal operator extension theory of dual pairs (Grubb, 1968). For a given Friedrichs system the existence of a boundary condition such that the problem is well-posed is shown, as well as a classification of all such boundary conditions.

On the Caffarelli-Silvestre extension approach to fractional powers in Banach spaces

Jan Meichsner (*TU Hamburg, Germany*)

17:30

Christian Seifert (*TU Hamburg, Germany*)

In [1] the authors attracted a lot of attention when describing the action of the fractional Laplacian $(-\Delta)^\alpha$, $\alpha \in (0, 1)$, on a function f in some function space using a solution u of the ODE

$$u'' + \frac{1 - 2\alpha}{t} u' = -\Delta u$$

in the aforementioned space. One has $u(0) = f$ which is why one can consider u as an extension of f and especially in the case of the Laplacian one may interpret u as a harmonic function in “ $\mathbb{R}^{n+2-2\alpha}$ ”. Until now many other authors [2, 3, 4] contributed by discussing the approach for general sectorial operators A instead of $-\Delta$. Still it was an open problem whether the approach works for all sectorial operators and whether the above introduced solution is actually unique. The talk aims to answer these questions.

- [1] L. Caffarelli and L. Silvestre, *An extension problem related to the fractional Laplacian*, Comm. Partial Differential Equations **32** (2007), no. 8, 1245-1260.
- [2] P. R. Stinga and J. L. Torrea, *Extension problem and Harnack’s inequality for some fractional operators*, Comm. Partial Differential Equations **35** (2010), no. 11, 2092-2122.
- [3] J. E. Galé, P. J. Miana and P. R. Stinga, *Extension problem and fractional operators: semigroups and wave equations*, Journal of Evolution Equations **13** (2013), no. 2, 343-368.
- [4] W. Arendt, A. F. M. ter Elst and M. Warma, *Fractional powers of sectorial operators via the Dirichlet-to-Neumann operator*, Comm. Partial Differential Equations **43** (2018), no. 1, 1-24.

The essential numerical range for unbounded linear operators

Sabine Bögli (*Imperial College London, United Kingdom*)

17:50

Marco Marletta (*Cardiff University, United Kingdom*)

Christiane Tretter (*Universität Bern, Schweiz*)

We study approximations of a linear Hilbert space operator T by projection methods or domain truncation methods. The eigenvalues of the approximating operators may accumulate at a point that does not belong to the spectrum of T . The occurrence of such a spurious eigenvalue is commonly known as spectral pollution. We introduce the concept of essential numerical range $W_e(T)$ for unbounded operators and study its fundamental properties including possible equivalent characterizations and perturbation results. Many of the properties known for the bounded case do not carry over to the unbounded case, and new interesting phenomena arise which we illustrate by some striking examples. A key feature of the essential numerical range $W_e(T)$ is that it captures spectral pollution in a unified and minimal way when approximating T by projection methods or domain truncation methods for PDEs. We present some interesting numerical examples.

The Crouzeix conjecture and deformations of the numerical range.

Patryk Pagacz (*Jagiellonian University, Poland*)

18:10

Pawel Pietrzycki (*Jagiellonian University, Poland*)

Michal Wojtylak (*Jagiellonian University, Poland*)

Crouzeix observed in [1] that for any operator A in a Hilbert space and any polynomial p

$$p(A) \leq C \sup_{W(A)} p$$

where $W(A)$ is the numerical range of A and the constant $C > 0$ is universal, i.e. does not depend neither on the operator nor on the space. He also proved in the same paper that $2 \leq C \leq 11.08$ and conjectured that $C = 2$. We will review recent developments on proving the conjecture ($C \leq 1 + \sqrt{2}$ in [2]) and show some deformations of the numerical range that lead to new constants. The talk is based on joint work with P. Pagacz and P. Pietrzycki. [1] Patryk Pagacz,

Paweł Pietrzycki and Michał Wojtylak. From the von Neumann inequality to the Crouzeix conjecture and further [2] Crouzeix, Michel. Numerical range and functional calculus in Hilbert space. *Journal of Functional Analysis* 244.2 (2007): 668-690. [3] Crouzeix, Michel, and César Palencia. The Numerical Range is a $(1 + \sqrt{2})$ -Spectral Set. *SIAM Journal on Matrix Analysis and Applications* 38.2 (2017): 649-655.

S23.03 | Applied operator theory

Date: February 20, 2019

08:30-09:30

Room: SR 06

Differential-algebraic operators and the Kronecker form

Timo Reis (*Universität Hamburg, Germany*)

08:30

Felix Schwenninger (*Universität Hamburg, Germany*)

Marc Puche (*Universität Hamburg, Germany*)

We consider constant-coefficient differential-algebraic equations from an operator theoretic point of view. We show that the Kronecker form allows to determine the nullspace and range of the corresponding differential-algebraic operators. This yields simple matrix-theoretic characterizations of features like closed range and Fredholmness.

Around maximal regularity with respect to L^∞

Felix Schwenninger (*Universität Hamburg, Germany, Bergische Universität Wuppertal, Germany*)

09:10

Birgit Jacob (*Bergische Universität Wuppertal, Germany*)

Jens Wintermayr (*Bergische Universität Wuppertal, Germany*)

A classic result by Baillon asserts that for a sectorial operator on a Banach space, maximal regularity with respect to continuous functions is equivalent to the following alternative: either A is bounded or the Banach space contains an isomorphic copy of c_0 . We show how this is linked with questions in the context of the continuity of mild solutions for inhomogeneous Cauchy problems arising in control theory (input-to-state stability) and discuss an extension of Baillon's result.

S23.04 | Applied operator theory

Date: February 20, 2019

14:00-16:00

Room: SR 03

Integration by parts on the law of the modulus of the Brownian bridge

Martin Grothaus (*TU Kaiserslautern, Germany*)

14:00

Robert Voßhall (*TU Kaiserslautern, Germany*)

We prove an infinite dimensional integration by parts formula on the law of the modulus of the Brownian bridge from 0 to 0. The main motivation for all this is the construction of an SPDE whose invariant measure would be the law of the reflecting Brownian bridge, a problem which is still open despite the recent fantastic advances in very difficult SPDEs, thanks to regularity structures and/or para-products. It seems that the SPDE which motivates this integration by parts formula is even more difficult than KPZ, since it contains a local time which is not covered by the new theories yet.

An agent based modeling of spatially inhomogeneous host-vector disease transmission

Wolfgang Bock (*TU Kaiserslautern, Germany*)

14:20

Torben Fattler (*TU Kaiserslautern, Germany*)

Isti Rodiah (*TU Kaiserslautern, Germany*)

In this talk we consider a microscopic model for the host-vector disease transmission based on configuration space analysis. We model transmission with a birth-death mechanism in the vector component and mobility in the host component. Our intention is to show that a Vlasov type scaling, which is a mean-field-like scaling of an interacting particle system, leads to the known equations used in epidemiology to model host-vector disease spread on the kinetic level. Configuration space analysis is here a very powerful tool. The concepts of harmonic analysis in this framework are used to derive first the dynamics of correlation functions - giving a hierarchical system of equations comparable to the well known BBGKY hierarchy in Hamiltonian dynamics. Then a proper Vlasov type scaling guarantees that the resulting Vlasov hierarchy is closed and possesses the property of preservation of chaos. The limiting system of time evolution equations is non-linear and strongly related to the well-known Fisher-KPP equations. A numerical analysis strengthens the analytical results. Moreover, the dynamics of case numbers over time gives qualitatively the solution of a SISUV-ODE system. The microscopic dynamics hence leads to the right behavior in the scaling limit.

Homogenization of abstract evolutionary equations via unfolding

Stefan Neukamm (*TU Dresden, Germany*)

14:40

Mario Varga (*TU Dresden, Germany*)

Marcus Waurick (*University of Strathclyde, UK*)

In recent years, it has been shown that a variety of evolutionary equations of mathematical physics share a common form, which can be described in a unified way by an abstract operator-theoretic Hilbert space framework. Recently homogenization strategies for sequences of such evolutionary equations have been established. In this talk we present a homogenization method that combines ideas from well-established abstract procedures with input from stochastic homogenization. In particular, the notion of stochastic two-scale convergence and stochastic unfolding are reconsidered in a general operator-theoretic context. As examples of the abstract homogenization result, we present homogenization of elliptic equations, Maxwell's equations and the wave equation.

Quantitative unique continuation principles and application to control theory for the heat equation

Martin Tautenhahn (*Technische Universität Chemnitz, Germany*)

15:00

Ivica Nakić (*University of Zagreb, Croatia*)

Matthias Täufer (*Technische Universität Dortmund, Germany*)

Ivan Veselic (*Technische Universität Dortmund, Germany*)

This talk is divided into two parts. In the first part we discuss a so-called scale-free and quantitative unique continuation principle for spectral projectors of Schrödinger operators. Let $\Omega = \Lambda_L = (-L, L)^d$ or $\Omega = \mathbb{R}^d$, and $H = -\Delta + V$ be a Schrödinger operator on $L^2(\Omega)$ with a bounded potential V . If $\Omega = \Lambda_L$ we impose Dirichlet, Neumann, or periodic boundary conditions. The unique continuation principle states that for any $E \geq 0$, and any $\phi \in \text{Ran } \chi_{(-\infty, E]}(H)$ we have

$$\|\phi\|_{L^2(\Omega)}^2 \leq C_{\text{sfuc}} \|\chi_{S_\delta \cap \Omega} \phi\|_{L^2(\Omega)}^2,$$

where $S_\delta \subset \mathbb{R}^d$ is a union of equidistributed δ -balls, and $C_{\text{sfuc}} = C_{\text{sfuc}}(d, E, \delta, \|V\|)$ some explicitly given constant.

In the second part of the talk we will discuss an applications thereof to control theory. On the time interval $[0, T]$ we consider the controlled heat equation

$$\partial_t u + Hu = f \chi_{S_\delta \cap \Omega},$$

where $u, f \in L^2([0, T] \times \Omega)$, and $u(0, \cdot) \in L^2(\Omega)$. Note that the control function f acts on the set S_δ only. Our aim is to study null-controllability in time $T > 0$, i.e. there is a control function f such that $u(T, \cdot) = 0$. We provide explicit and sharp estimates on the costs of the form $\|f\|_{L^2([0, T] \times \Omega)} \leq C \|u_0\|_{L^2(\Omega)}$.

The Tan 2Theta-theorem in fluid dynamics

Luka Grubisic (*University of Zagreb, Croatia*)

15:20

Vadim Kostrykin (*Johannes Gutenberg-University Mainz, Germany*)

Konstantin A Makarov (*University of Missouri, USA*)

Stephan Schmitz (*University of Koblenz-Landau, Germany*)

Kresimir Veselic (*Fernuniversität Hagen, Germany*)

We show that the generalized Reynolds number (in fluid dynamics) introduced by Ladyzhenskaya is closely related to the rotation of the positive spectral subspace of the Stokes block-operator in the underlying Hilbertspace. We also explicitly evaluate the bottom of the negative spectrum of the Stokes operator and prove a sharp inequality relating the distance from the bottom of its spectrum to the origin and the length of the first positive gap.

S23.05 | Applied operator theory

Date: February 20, 2019

16:30-18:30

Room: SR 03

Perturbation of positive semigroups

András Bátkai (*Pädagogische Hochschule Vorarlberg, Austria*)

16:30

We present new perturbation results for positive semigroups along with applications. An important question under investigation will be the behaviour of the spectral properties under perturbation.

Reference:

Bátkai, A., Kramar-Fijavž, M., Rhandi, A., “Positive Operator Semigroups: from finite to infinite dimensions”, Operator Theory: Advances and Applications 257, Birkhäuser Verlag, 2017, ISBN 978-3-319-42811-6

Orthogonality and selfadjointness for extensions of inner products

Christian Wyss (*Universität Wuppertal, Germany*)

16:50

Let V, V_0 be two Hilbert spaces such that $V \subset V_0$ with dense and continuous imbedding. Let $[\cdot, \cdot]$ be a (possibly indefinite) inner product on V , not necessarily the Hilbert space inner product. We study the case where this inner product can be extended in such a way that $[vw]$ is also defined for $v \in V_1, w \in V_0$, where the Hilbert space $V_1 \subset V$ is the dual of V_0 with respect to $[\cdot, \cdot]$. Using this extension, geometric notions related to the inner product $[\cdot, \cdot]$ on V can be

generalised to objects living in the bigger space V_0 . We consider e.g. the orthogonal complement of a subspace $U \subset V_0$ and the notion of selfadjointness of an operator T_0 on V_0 with $D(T_0) \subset V_1$, both with respect to the extended inner product. We obtain results which are analogous to the Krein space situation. The theory can be applied to the Hamiltonian operator matrix from systems theory.

Riesz bases and controllability for port-Hamiltonian systems

Birgit Jacob (*Bergische Universität Wuppertal, Germany*)

17:10

Julia Kaiser (*Bergische Universität Wuppertal, Germany*)

Riesz bases are a generalization of orthonormal bases. More precisely, a sequence of vectors in a Hilbert space H is a Riesz basis for H if there exists a boundedly invertible operator S such that the image of the sequence under the operator S is an orthonormal basis of H . We consider a special kind of hyperbolic partial differential equations on a one dimensional spatial domain. In particular, we are interested in partial differential equations which can be formulated using a Port-Hamiltonian operator of order 1. This class includes wave equations, for example. We aim to find an answer to the question whether such a port-Hamiltonian operator possesses a Riesz basis consisting of eigenvectors. In this talk we present necessary and sufficient conditions guaranteeing that a port-Hamiltonian operator of order 1 possesses a Riesz basis consisting of eigenvectors. Furthermore, we prove that every port-Hamiltonian system of order 1 is exactly controllable.

Solvability of the inhomogeneous Cauchy-Riemann equation for weighted smooth vector-valued functions

Karsten Kruse (*TU Hamburg, Germany*)

17:30

We derive sufficient conditions for the surjectivity of the Cauchy-Riemann operator between spaces of weighted smooth Fréchet-valued functions.

This is done by establishing an analog of Hörmander's theorem on the solvability of the inhomogeneous Cauchy-Riemann equation in a space of smooth complex-valued functions whose topology is given by a family of weights. The proof relies on local solvability in combination with the Mittag-Leffler procedure.

Using tensor products, we deduce the corresponding result on the solvability of the inhomogeneous Cauchy-Riemann equation for Fréchet-valued functions.

S24 | History of mechanics and history, teaching and popularization of mathematics

Organiser: Dietmar Gross (*Technische Universität Darmstadt, Germany*)
Otto T. Bruhns (*Ruhr-University Bochum, Germany*)

S24.01 | History of mechanics and history, teaching and popularization of mathematics

Date: February 19, 2019
Room: SR 05

16:30-18:30

Science thriller: The dramatic destiny of Alexander Mohrenstein-Ertel and the history of elasto-hydrodynamics

Elena Popova (*Technische Universität Berlin, Germany*)
Valentin L. Popov (*Technische Universität Berlin, Germany*)

16:30

Presentation is devoted to the life and work of Alexander Mikhailovich Ertel, the founder of elasto-hydrodynamics. He was the first to solve problems of hydrodynamic lubrication accounting for elastic deformation of the bodies in contact as well as for the dependence of the viscosity of the lubricant on pressure and temperature, thereby opening a new branch of tribology - elasto-hydrodynamics. However, due to complicated historical entanglements, the real authorship remained unknown over many years. We investigate the circumstances of the creation of elasto-hydrodynamics and provide a short sketch of the main ideas of Mohrenstein-Ertel. The biography of Mohrenstein-Ertel is like a criminal novel: the 20th century history is reflected in the hard fate of this scientist and Russian history up to the time of Pushkin can be traced in his genealogy. Already during his student years, Alexander Ertel recognized the crucial importance of three factors in lubrication: cavitation, elastic deformation of contacting partners, and pressure and temperature dependence of viscosity of the lubricant. He not only studied these factors in their interrelation but also applied and patented them. In the Soviet Union, he enjoyed recognition of such famous scientists as P.L. Kapitza and M.M. Khrushchov. After his escape to West Germany, he had to start his carrier from the beginning. With his changed identity, he could not claim for years the authorship of his fundamental results in elasto-hydrodynamics. However, his results have not been lost: through Grubin's publication, they became known to the scientific community, and significantly influenced the development of tribology. In West Germany, he continued his work by practical implementation of the above three ideas. Alexander Mohrenstein-Ertel was lucky to survive a severe illness and a severe car accident. He was lucky to see his ideas implemented in industrial practice. He could reveal his identity after the Stalin's death, and could witness the recognition of his contribution through the German Tribological Society and international tribological community.

This presentation is based on the works of Alexander Mohrenstein-Ertel, memories of colleagues as well as very exciting and informative conversations with Michael Mohrenstein-Ertel, the son of Alexander Mohrenstein-Ertel and his granddaughter, Marina Ertel.

References

[1] E. Popova, V. L. Popov, On the history of elasto-hydrodynamics: The dramatic destiny of Alexander Mohrenstein-Ertel and his contribution to the theory and practice of lubrication, ZAMM - Journal of Applied Mathematics and Mechanics, 95, 652-663 (2014)

August Wöhler - founder of fatigue strength

Harald Zenner (*TU Clausthal, Germany*)

17:10

Karsten Hinkelmann (*Volkswagen, Germany*)

August Wöhler was an interesting and unique character, influenced by the 19th century industrial revolution, especially railway development. The spread of this new technology caused numerous problems. Fractures arose on axles, wheels and rails at stresses below the component's static fracture strength. There was no scientific explanation for this. August Wöhler was able to prove by systematic tests that repeated, thus dynamic stresses far below the static strength may lead to fracture.

In the field of technology, good biographies are relatively rare. Except for those written by individuals referring to personal acquaintance, most facts get lost. For A. Wöhler, there are two very authentic biographies. The first biography was published in 1914, the year of August Wöhler's death. It is by L. Troske, a former employee of A. Wöhler. The second biography was published in 1918 by Wöhler's grandson R. Blaum. A short overview about Wöhler's curriculum vitae with important life stages will be given.

Wöhler's fatigue tests running over a time of fourteen years had led to five publications between 1858 and 1870. Wöhler, to be sure, was not the first who carried out fatigue tests. But he is internationally regarded as the first who studied parameters of dynamic strength methodically. Wöhler had to invent his testing machines by himself and set a precedent thereby. He is considering not only the endurance limit but also constructions for a limited number of cycles in use. His experimental studies meant a lot to August Wöhler. But also very important for him was the reliable strength dimensioning by an exact determination of the allowable stress, a classification of materials (iron and steel) regarding rather characteristic properties than application and the constitution of independent testing institutions, the institutes for materials research and testing. Both his achievements as well as criticism are presented. For example A. Wöhler did not graph his own results. This has only been done by his successor L. Spangenberg in a linearly scale. The double logarithmic plot was not used before 1910 by O. H. Basquin. Furthermore there is no single passage drawing a comparison between the fracture surfaces in the test and those in operation. All this, however, cannot diminish its achievements.

Palmgren, Gaßner and the challenges of fatigue at variable amplitudes

Michael Wächter (*TU Clausthal, Germany*)

17:30

Karsten Hinkelmann (*TU Clausthal, Germany*)

Alfons Esderts (*TU Clausthal, Germany*)

Harald Zenner (*TU Clausthal, Germany*)

While the preceding presentation by Zenner and Hinkelmann deals with fatigue strength at constant amplitudes, this contribution, which begins in the 1920s, gives an overview over early developments in the field of fatigue strength under variable amplitudes, which means load spectra. Considerations on how to determine the strength or service life at variable amplitudes based on the strength at constant amplitudes were first published by Palmgren in 1924. He assumes that partial damage can be calculated from the number of applied and bearable cycles at one load level. If partial damages of different load levels are summed, the total damage and thus the bearable service life of the component under consideration can be calculated. Later, Langer (1937) and Miner (1945) came up with the same idea probably independently of each other and also independently of Palmgren's work. Nowadays, the described idea is mainly attributed to Miner (Miner's rule) - actually, modifications of the original rule are used. The limitations formulated by the inventors and the comparisons made with experiments at that time are to be presented.

Testing at variable amplitudes is closely linked to Ernst Gaßner, who carried out the first variable amplitude test in 1938. The test technique of that time did not yet permit an actually random mixing of the amplitudes of a load spectrum; instead, Gaßner carried out block program tests in which the amplitudes of the spectrum to be tested were combined in blocks of constant amplitude and tested one after the other.

From about 1960 onwards, Gaßner and Lipp systematically tried to compare the results from block program tests with those from real service loads. Therefore, they mounted a small specimen test bench in the trunk of a VW Beetle and coupled the load transmission to the rear axle of the vehicle so that the real loads were transferred to the specimens while the vehicle was in motion. Through the development of servo-hydraulic test equipment in the 1960s and 1970s, which made it possible to change load amplitudes cycle by cycle and thus to achieve a more realistic mixing or actual time functions. The weaknesses of block program tests and linear damage accumulation were discovered in this way, e.g. by the contributions of Jacoby. As a result, more and more modifications have been developed to date, while the complex damage process is still the subject of numerous investigations.

A brief historical tour of glacier ice on earth and its role in climate dynamics

Kolumban Hutter (*ETH Zürich, Switzerland*)

17:50

Dietmar Gross (*TU Darmstadt, Germany*)

The study of glacier ice started with observations of the dynamics of Alpine glaciers. A ladder, left in 1788 at the ice-fall of the Col-de-Géant by Forbes was 44 years later found at the three-glacier merge of the Mère de Glace. Hugi and Agassi measured the motion of rocks on the middle moraine. Forbes and Tyndall found that velocities of glacier objects are larger on the glacier surface than at depth and larger in the middle of the glacier-width than close to the boundaries, as reported by Helmholtz (1865). On this basis Rendu & Forbes identified similarities of glacier flows with streams of very viscous fluids. It was 1950s when physicists postulated the constitutive equation for isotropic ice as power law fluid (Nye 1952) that was verified by Glen (1953) and Steinemann (1958). Various second grade fluid alternatives provide corrections at relatively high costs of mathematical-numerical complexities.

Large-scale ice IBVPs are viscous, heat conducting Stokes problems, which may involve cold ice regions with the ice temperature below melting, separated by a class I mixture of ice with water inclusions. The dynamics of the cold-temperate transition surface between the two regions is governed by a Clausius-Clapeyron equation.

At the surface, snow accumulation and radiative heat must be parameterized or these quantities must be taken over from concurrent GCMs of the atmosphere. Similarly, for the ice-ocean interface on floating portions. Here, general ocean-circulation models are operative. At the ice-shelf front, mass-loss by calving must be parameterized, important for marine glaciers and ice-shelves in GCM scenarios. The theoretical parts of these IBVPs have kept glacio-climatologists busy since the 1980s. Yet, to integrate the Stokes problem computationally is still out of reach at today's CPU times.

It was very early realized that the full Stokes model must be simplified. To obtain it, perturbation methods were employed. It led to the shallow-ice and shallow-shelf approximations (SIA, SSA). Today, there exist several open-source programs that solve the Stokes formulations for small scale SIA and SSA problems and whole global analyses. The scientific reports are concerned e.g. with the deglaciation of the mountainous glaciers, the ice loss of Greenland, West Antarctica, coupled with sea level rise, affecting the global circulation of the ocean currents and the Earth's climate and leading to millions of displaced people.

S24.02 | History of mechanics and history, teaching and popularization of mathematics

Date: February 20, 2019

08:30-09:30

Room: SR 05

Reconstruction of the genesis of a renaissance algorithm to calculate sine tables

Peter Ullrich (*Universität Koblenz-Landau, Germany*)

08:30

Jost Bürgi (1552-1632) is known as creator of astronomical clocks and scientific instruments and as author of one of the first tables for logarithms. Recently, Menso Folkerts has discovered an up to then unpublished manuscript in which Bürgi presents an algorithm to calculate also sine tables of high precision with only a modest amount of numerical effort [1], [2].

Several modern proofs for the correctness of this algorithm have been given: In [1] and [6] the power method for determining eigenvalues is used that was published by Pollacek-Geiringer and von Mises in 1926. In [3] discrete Fourier transforms come into play. All these methods, however, were not at hand at Bürgi's time. One may, of course, assume that Bürgi himself had no proof [4, p. 8].

But even if Bürgi was not in possession of a formal proof fulfilling modern standards, there must have been a way how he had found his algorithm. Furthermore, he will have convinced himself (even if only on numerical evidence) that it leads to correct results: The calculations were only an auxiliary means for him to construct his costly devices, and he will not have used a tool that would not function assuredly.

Building on previous results [5], the contribution will present an educated guess how Bürgi may have found his algorithm and also collected enough evidence for its correctness. For this, only methods are needed which were known at Bürgi's time, like prosthaphaeresis and the false position method.

Literatur

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Using computer simulations in lectures in mathematics and in the natural sciences: learning-theoretical justifications

Roland Gunesch (*PH Vorarlberg, Austria*)

08:50

Every applied mathematician knows the value of computer simulations for conducting applied research. In education (especially university teaching) computer simulations are also increasingly

used. This talk presents an overview of results from the mathematics education literature about the usefulness of using computer simulations in lectures. Therefore, this talk justifies (some) established teaching practices in mathematics lectures.

Some computer simulations (both very new ones and ones which have been used for a while for educational purposes) from various areas of mathematics and natural sciences are presented in this talk, along with ideas of how to use them in lectures and with an analysis of their advantages and possible shortcomings.

This talk explains some concepts of the theory of analysis of simulations from a learning-theoretical point of view, such as the instructional principles of multimedia learning (Mayer, 2009) and cognitive load theory (Chandler & Sweller, 2000).

The talk presents various concrete reasons why computer simulations can improve lectures, such as the use of realistic learning environments, active and constructive learning and deep understanding via computer simulations (Gräsel, Bruhn, Mandl & Fischer, 1997), complex problem solving with computer simulations (Tennyson & Breuer, 2002), the ability to repeat experiments in computer simulations and resulting knowledge (White & Frederiksen, 1998, 2000), students' ability to form their own hypotheses and test them with computer simulations (Klahr & Dunbar, 1988; White & Frederiksen, 1998), discovery learning and its use in the natural sciences (Hammer, 1997; Swaak & de Jong, 1996), increased motivation of students due to the interactivity of computer simulations (Lindström, Marton & Ottoson, 1993; Strzebkowski & Kleeberg, 2002; Swaak & de Jong, 1996; Haack, 1997).

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