gacm German Association for Computational Mechanics

TU WIEN TECHNISCHE UNIVERSITÄT WIEN

10th GACM

Colloquium on Computational Mechanics

for Young Scientists from Academia and Industry

September 10 to 13, 2023
Vienna, Austria

Contents

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Last update: September 10, 2023

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Organization

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Key, Fabian	TU Wien
De Paoli, Marco	TU Wien & University of Twente
Wagner, Antonia	TU Wien
Stender, Merten	TU Berlin

Hosting Institutes

Institute of Lightweight Design and Structural Biomechanics

Faculty of Mechanical and Industrial Engineering

Gumpendorfer Straße 7,
A-1060 Vienna,
Austria

Institute of Fluid Mechanics and Heat Transfer

Faculty of Mechanical and Industrial Engineering

Getreidemarkt 9,
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Institute of Mechanics of Materials and Structures

Faculty of Civil and Environmental Engineering

Karlsplatz 13,
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Zonta, Francesco	TU Wien	Fluid Mechanics and Heat Transfer
Zwicke, Florian	TU Wien	Lightweight Design and Structural Biomechanics

Venue

The conference will be held on the campus of TU Wien. The main program takes place at Campus Gußhaus (C), which is located in Gußhausstraße 25-29. See also the Maps.

Welcome by the Organizers

Dear Participants,

We are excited to welcome you to the **10th GACM Colloquium on Computational Mechanics for Young Scientists from Academia and Industry 2023** at TU Wien. We are pleased that you came to Vienna and proud to offer you a conference that is certified as a sustainable event! It is jointly hosted by the Institutes of Lightweight Design and Structural Biomechanics, Fluid Mechanics and Heat Transfer, and Mechanics of Materials and Structures.

The GACM Colloquium brings together young researchers in the field of computational mechanics. It provides excellent opportunities for students and postdocs to present their work, acquire new knowledge in the field of numerical modeling in engineering and science, and establish a network of colleagues and peers. The colloquium consists of 21 minisymposia – organized by selected young scientists – as well as a poster session and six plenary lectures. We are thrilled that so many of you responded to the call and submitted their contributions or organized minisymposia.

We are truly grateful to everyone who invested their time to make this conference a success. We want to express our gratitude to all staff members who supported us in our mission to make this colloquium a fruitful and memorable event that helps shape the careers of the next generation of researchers in computational mechanics.

We wish everyone a pleasant stay in Vienna, full of productive discussions and interesting presentations.

The conference chairpersons

Fabian Key
Marco De Paoli
Antonia Wagner
Merten Stender

Welcome by the GACM President

As GACM president, and in the name of the entire board, it is a great pleasure for me to welcome you all to this year's GACM Colloquium for Young Scientists from Academia and Industry. We thank especially the TU Wien for hosting this event, and the organizers – Fabian Key, Marco De Paoli, Antonia Wagner, and Merten Stender.

I am so grateful that they stepped in, after the necessary delay of the in-person 2021 meeting (held in Essen in 2022), to organize the current colloquium only at a year's notice and thus bring us back to the bi-annual schedule where the colloquium is held in the odd years, alternating with major ECCOMAS and IACM conferences.

And regardless of the circumstances, the first glance at the program shows a very innovative event. The certification for sustainability, the plenaries that involve the rising stars in our community, the unique social program, are just a few aspects. The organizers invested an incredible amount of energy and creativity preparing the colloquium, and now it's up to all of us to make the best of it.

Vienna holds a special place in the development of the computational mechanics community. The 5th World Congress of the IACM was held here in 2002, The 15 years of ECCOMAS were celebrated in Vienna in 2008, and the ECCOMAS Congress in 2012 has certainly left a lasting impression. I am sure that the GACM colloquium will be similarly appreciated by all participants.

The year 2023 has been hard on our community, marked by passing of some of the pioneers, such as Ivo Babuška, and very recently, Tinsley Oden. These persons should inspire us, and motivate us to do our best in the interdisciplinary and collaborative endeavor that is the computational mechanics. A lively discussion and exchange of scientific ideas is an integral part of our efforts, and the GACM colloquium is an ideal platform.

Marek Behr

Plenary Speakers

Dr. Dirk Hartmann, Siemens Digital Industries Software

Executable Digital Twins -
Integrating the digital and real world

Monday, 11 Sept, 9:10 am – 9:55 am

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Prof. Alexander Popp, UniBW München

Scalability of Nonlinear Problems in Contact Mechanics and Mixed-Dimensional Coupling - From Computational Strategies to Multigrid Solvers

Monday, 11 Sept, 9:55 am – 10:40 am

Prof. Sebastian Schöps, TU Darmstadt

Isogeometric Mortar Methods for Electromagnetism

Tuesday, 12 Sept, 11:10 am – 11:55 am

Prof. Jelena Ninic, University of Birmingham

Application of machine learning and computer vision for decision making support during the infrastructure lifecycle

Tuesday, 12 Sept, 11:55 am – 12:40 am

Prof. Liesbet Geris, University of Liège and KU Leuven

In vitro, in vivo, in silico: use of computer modeling and simulation in skeletal pathologies and treatment

Wednesday, 13 Sept, 11:10 am – 11:55 am

Dr. Ivo Steinbrecher, UniBW München

Mixed-dimensional finite element formulations for beam-to-solid interaction

Wednesday, 13 Sept, 11:55 am – 12:40 am

Minisymposia

MS 01: ANN and data-driven approaches in material and structural mechanics
Yousef Heider, Fadi Aldakheel, Franz Bamer, Henning Wessels, Karl A. Kalina

MS 02: Current trends in modelling and simulation of biological systems: numerics, application and data integration
Christian Bleiler, Sebastian Brandstaeter, Lena Lambers, Renate Sachse

MS 03: (merged with MS 17) Computational Modeling and Methods for Multiphase Problems
Leonardo Boledi, Benjamin Terschanski, Donat Weniger

MS 04: Digital Twins and Their Enabling Technologies
Max von Danwitz, Norbert Hosters

MS 05 Multi-scale modelling and computational approaches to continua with micro-structure
Adam Sky, Andreas Warkentin, Stephan Lange

MS 06: Multiphysical Modeling of Complex Material Behavior
Matthias Rambausek, Elten Polukhov, Miguel A. Moreno-Mateos, Markus Mehnert

MS 07: (canceled) Modeling and discretization of slender continua and their interaction
Ivo Steinbrecher, Christoph Meier, Christian Hesch, Joachim Linn

MS 08: Numerical simulations of flows in porous media
Marco De Paoli

MS 09: Multi-scale Shape Optimization Problems in Continuum Mechanics
Ramy Nemer, Daniel Wolff, Jacques Zwar

MS 10: Computational treatment of slender structures allowing for large rotations
Alexander Müller, Rebecca Thierer, Lisa Julia Nebel

MS 11: Stratified turbulence
Francesco Zonta

MS 12: Modeling and Simulation of Heterogeneous Materials: Microstructure and Properties
Markus Sudmanns, Yejun Gu

MS 13: Droplets, bubbles and interfaces in turbulent flows
Mahdi Saeedipour, Francesca Mangani

MS 14: Mechanics of soft multifunctional materials: Experiment, modeling and simulation
Mokarram Hossain, Daniel Garcia-Gonzalez, Matthias Rambausek

MS 15: (canceled) Modeling of fiber-based products
Ann-Malin Schmidt, Daniela Sofronova

MS 16: Modeling, Simulation and Quantification of Polymorphic Uncertainty in Real Word Engineering Problems
F. Niklas Schietzold, Selina Zschocke

MS 17: (merged with MS 03) Multi-Phase and Interface Flow Problems
Patrick G. Antony, Blanca Ferrer Fabón, Norbert Hosters

MS 18: (canceled) The role of interphases and interfaces in the overall behavior of composites
Paras Kumar, Soheil Firooz

MS 19: Integrating Computational and Experimental Mechanics
Knut Andreas Meyer, Tobias Kaiser

MS 20: Reduced order modeling and fast simulation strategies
Margarita Chasapi, Thibaut Hirschler

MS 21: General
This session is intended for submissions that do not fall into the scope of any of the scheduled minisymposia.

General Information

Social Events

Riddle Rally City Tour

CityRiddler is offering a unique riddle rally to explore the city of Vienna. Get to know attendees from the colloquium, solve riddles, and explore the hidden gems of Vienna together. Do you know the Freemason headquarters in Vienna? Or the story of the street of blood? Can you solve the secret equation at the staff that lies in iron? In the CityRiddler rally, you join a team with up to 6 people and explore the secret spots of the inner city of Vienna with your smartphone. For more information visit www.cityriddler.com.

Viator – Tripadvisor company

Location: start at Karlsplatz in front of Karlskirche, 1040 Wien

Time: Sunday, September 10, 2023, starting 15:00

Welcome Reception

After participating in the city tour or arriving in Vienna, the Welcome Reception offers a wonderful opportunity to socialize over a cool drink and a light snack.

NMPB Architekten + Arch. Neumayr: Umbau TU Wien – © TU University 2015

Location: Kuppelsaal (4th floor), TU Wien main buidling, Karlsplatz 13, 1040 Wien

Time: Sunday, September 10, 2023, starting 19:00

Sparkling Moments on the Museum's Roof

You will be offered an entertaining and informative insight into the Museum of Natural History (NHM) Vienna. You will take a look behind the scenes of the museum's world-class collections and find out how and on what the staff at the NHM Vienna is carrying out research. The tour concludes with a glass of sparkling wine on the roof terrace overlooking the city center.

Credits: Miguel Mendez from Malahide, Ireland, CC BY 2.0

Location: Museum of Natural History (NHM Museum), Burgring 7, 1010 Wien

Time: Monday, September 11, 2023, starting 18:30

Conference Dinner

The main social event of the conference, the conference dinner, will take place in the Rathauskeller, the restaurant located at the Vienna City Hall. A sustainable dinner will be served in this beautiful historical building located in the heart of Vienna.

© WienTourismus/Christian Stemper

Location: Wiener Rathauskeller, Rathauspl. 1, 1010 Wien, Austria

Time: Wednesday, September 13, 2023, starting 18:30

Coffee Breaks

Coffee breaks will take place in Aula, at campus Gußhaus (C).

Lunch Breaks

Lunch on all three days of the event is included in the conference fee. Lunch breaks will take place in Aula, at campus Gußhaus (C).

Poster Session

A poster session is scheduled for Monday, September 11, 15:20 – 16:10 in Aula, where also the coffee breaks and lunch breaks will take place. There will be three Best Poster Awards, including prize money, selected by a committee of referees. The awards will be announced during the conference closing.

Wi-Fi

Wi-Fi will be available during the conference. Details on how to access can be found on the inside of your name tag.

Information for Speakers

Please arrive at the session on time and, if possible, introduce yourself to the session chair so that one can ensure that all speakers are present. The time allocated for each speaker is 20 minutes, including questions from the audience and setup of your laptop. You will have to use your own computer and connect via HDMI. Staff members will be available to help with any technical difficulties. To ensure that sessions start reliably at the scheduled time, session chairs are asked to strictly adhere to the schedule.

Information for Presenting a Poster

During an extended coffee break, the poster session will be held on Monday, September 11, from 15:20 to 16:10 (cf. the conference program). Poster presenters are asked to set up their posters prior to the session and to be present beside their posters during the session for discussions and answering questions. Please print your poster in advance and bring it with you to the venue as we do not have poster printing facilities on site. Note that the maximum poster size is DIN A0 portrait (841 x 1189 mm). Poster boards and mounting materials will be provided. Posters can be taken down after the coffee break on Wednesday afternoon (September 13, 15:00–15:30). Please note that all remaining posters will be removed and disposed of by the conference staff.

Sustainability

Certification

Our event obtained the certificate ÖkoEvent issued by the City of Vienna. In order to be granted such a certificate, a number of criteria need to be fulfilled, all of them designed to decrease the use of resources or the amount of waste and emissions. Measures that need to be implemented for an oekoevent include, e.g., the use of non-disposable products or the replacement of printed material with digital alternatives. This not only means higher standards and better quality for the participants, but also reflects positively on the outside view of the conference in general.

Travel and Mobility

To reach Vienna, there exist many convenient train connections. Furthermore, the conference will take place in one of the downtown campuses of TU Wien, located close to the central square Karlsplatz; a nearby transportation hub. Thus, the venue can be reached perfectly by public transport. Generally, the excellent public transportation system in Vienna will allow you to get around easily within the city. Another possibility to explore the city is provided by the public bike sharing service WienMobil Rad. In summary, Vienna offers many options for traveling with low emissions, which suits well the sustainable focus of the conference.

Sustainable Organic Catering

We are pleased to announce that the catering of the Welcome Reception and the daily coffee and lunch breaks will be delivered by the company Gaumenfreundinnen. The Gaumenfreundinnen live sustainability on all levels, which means: sustainable eat & drink, sustainable work, and sustainable business. They, therefore, fit perfectly into the concept of our event. The following points make up their offer and thus contribute to a sustainable catering:

100% Organic and 100% Meatless For food and beverages, Gaumenfreundinnen rely on an organic full-range offering, from the basic products to the smallest ingredient. Furthermore, the food offer is exclusively vegetarian or vegan.

Seasonal Ingredients and Regional Products Seasonal cuisine reduces the ecological footprint. That's why they vary their food offerings as much as possible with freshly harvested ingredients according to the season. In addition, regional procurement shortens delivery routes, saves C02, and promotes the local economy.

Reusable Tableware, Recycling, and Second-Hand Equipment Gaumenfreundinnen use only reusable, returnable tableware and place a high value on sustainable, recyclable packaging materials. Reusing helps to conserve natural resources. Therefore, their work equipment comes from second-hand sources wherever possible.

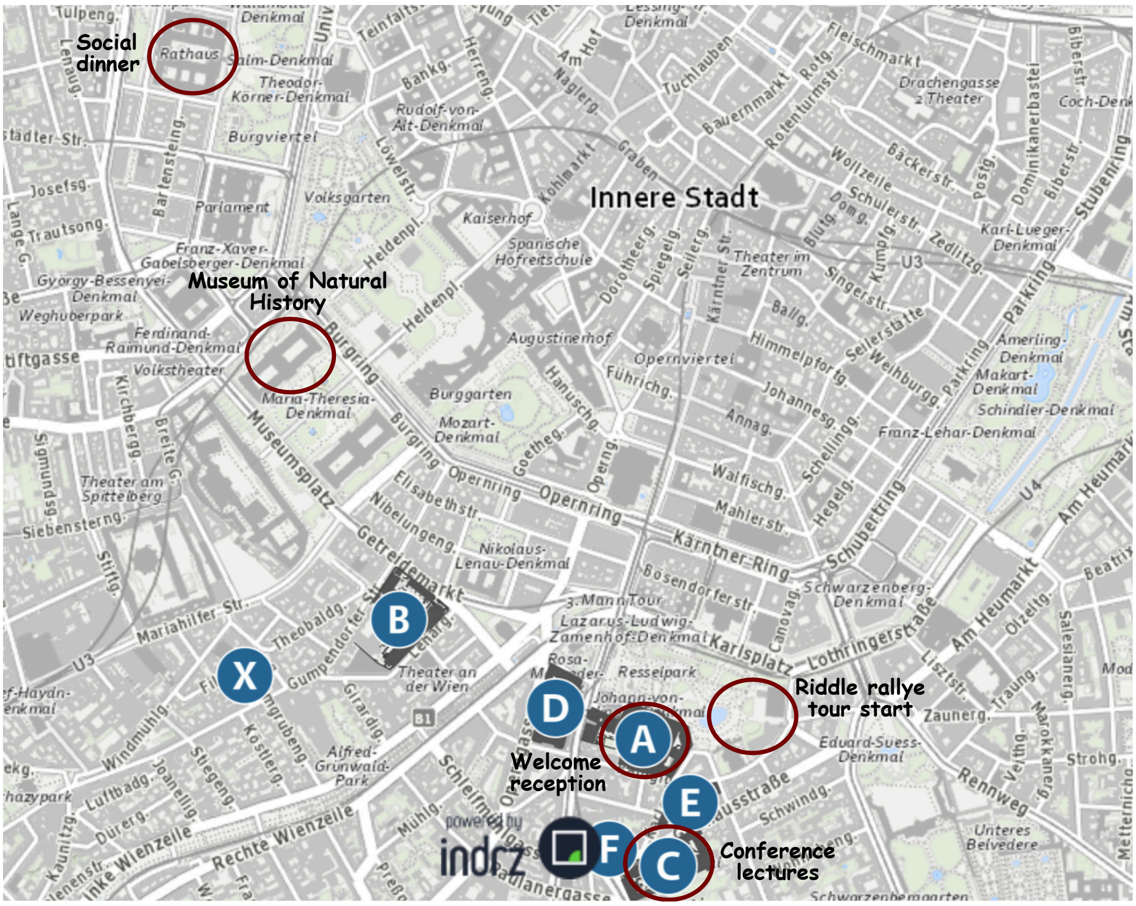
E-Mobility and Green Electricity They protect the environment wherever they are - with electricity from renewable energies and, since 2023, also with an e-vehicle.

Foodsharing is Caring Nothing ends up in the trash unnecessarily. And if something should be left over, they cooperate with the association Foodsharing Wien.

Mindful Company and Social Responsibility All the values they represent to their customers are naturally also lived out in their own corporate culture. The company Gaumenfreundinnen is managed by two women and maintains a socially responsible personnel policy at all levels.

Maps

Gußhausviertel
Karlsgasse
Gußhausstraße
Favoritenstraße
FA
CA
CB
CC
CD
CE
CF
CG
CH
EI7
EI8
EI9
EI10
powered by
indrz



Social dinner
Rathaus
Museum of Natural History
Innere Stadt
Parlament
Volksgarten
Burgviertel
Burggarten
Opernring
Kärntner Ring
Karlsplatz
Resselpark
Welcome reception
Riddle rallye tour start
Conference lectures
A
B
C
D
E
F
X
powered by
indrz

Timetable

The detailed program is available here.

MS: Minisymposium Talk, PL: Plenary Talk, Po: Poster contribution.

Sunday, September 10

15:00–17:00	**Riddle Rally City Tour**		
18:00–20:00	**Registration**		
19:00–20:30	**Welcome Reception**		

Monday, September 11

8:00–8:40	**Registration**		
8:40–9:10	**Opening Ceremony**		
9:10–9:55	PL	**Dirk Hartmann** Executable Digital Twins - Integrating the digital and real world	El7
9:55–10:40	PL	**Alexander Popp** Scalability of Nonlinear Problems in Contact Mechanics and Mixed-Dimensional Coupling - From Computational Strategies to Multigrid Solvers	El7
10:40–11:10	**Coffee Break**		
11:10–12:30	MS	**MS02-1** Biological systems **MS03** Phase-transition problems **MS05-1** Continua with micro-structure **MS20-1** Reduced order modeling and fast simulation strategies	El8 El10 El9 El7
12:30–13:40	**Lunch**		
13:40–15:20	MS	**MS02-2** Biological systems **MS05-2** Continua with micro-structure **MS11-1** Stratified turbulence **MS20-2** Reduced order modeling and fast simulation strategies	El8 El9 El10 El7
15:20–16:10	Po	Coffee Break & Poster Session	Aula
16:10–17:10	MS	**MS10-1** Slender structures allowing for large rotations **MS11-2** Stratified turbulence **MS12-1** Modeling and simulation of heterogeneous materials **MS20-3** Reduced order modeling and fast simulation strategies	El8 El10 El9 El7
18:30–19:30	**Sparkling Moments on the Museum's Roof**		

Tuesday, September 12

9:00–10:40	MS	**MS06-1** Multiphysical modeling of complex material behavior **MS10-2** Slender structures allowing for large rotations **MS12-2** Modeling and simulation of heterogeneous materials **MS13** Droplets, bubbles and interfaces in turbulent flows	EI7 EI8 EI9 EI10
10:40–11:10	**Coffee Break**		
11:10–11:55	PL	**Sebastian Schöps** Isogeometric mortar methods for electromagnetism	EI7
11:55–12:40	PL	**Jelena Ninic** Application of machine learning and computer vision for decision making support during the infrastructure lifecycle	EI7
12:40–13:40	**Lunch**		
13:40–15:20	MS	**MS01-1** ANN and data-driven approaches in mat. & struct. mech. **MS06-2** Multiphysical modeling of complex material behavior **MS19-1** Integrating computational and experimental mechanics **MS21-1** General	EI9 EI7 EI8 EI10
15:20–15:50	**Coffee Break**		
15:50–17:50	MS	**MS01-2** ANN and data-driven approaches in mat. & struct. mech. **MS06-3** Multiphysical modeling of complex material behavior **MS19-2** Integrating computational and experimental mechanics **MS21-2** General	EI9 EI7 EI8 EI10

Wednesday, September 13

9:00–10:40	MS	**MS09-1** Multi-scale shape optimization in continuum mechanics **MS16-1** Polymorphic uncertainty in engineering problems	EI7 EI9
10:40–11:10	**Coffee Break**		
11:10–11:55	PL	**Liesbet Geris** In vitro, in vivo, in silico: use of computer modeling and simulation in skeletal pathologies and treatment	EI7
11:55–12:40	PL	**Ivo Steinbrecher** Mixed-dimensional finite element formulations for beam-to-solid interaction	EI7
12:40–13:40	**Lunch**		
13:40–15:00	MS	**MS04-1** Digital twins and their enabling technologies **MS09-2** Multi-scale shape optimization in continuum mechanics **MS14-1** Mechanics of soft multifunctional materials **MS16-2** Polymorphic uncertainty in engineering problems	EI10 EI7 EI8 EI9
15:00–15:30	**Coffee Break**		
15:30–16:30	MS	**MS04-2** Digital twins and their enabling technologies **MS08** Numerical simulations of flows in porous media **MS09-3** Multi-scale shape optimization in continuum mechanics **MS14-2** Mechanics of soft multifunctional materials	EI10 EI9 EI7 EI8
16:30–16:40	**Short Break**		
16:40–17:40	**Closing**		
18:30–22:00	**Conference dinner**		

Partner Institutions and Sponsors

The organizers of the GACM 2023 would like to thank the following sponsoring and supporting organizations:

Sponsors

List of Abstracts

Plenary Lectures

Executable Digital Twins - Integrating the digital and real world

Dirk Hartmann PL

Siemens Digital Industries Software, Germany

We live in a world of exploding complexity with enormous challenges. Digital twins, tightly integrating the real and the digital world, are a key enabler for decision making in the context of complex systems. While the digital twin has become an intrinsic part of the product creation process, its true power lies in the connectivity of the digital representation with its physical counterpart.

To be able to use a digital twin scalable in this context, the concept of an executable digital twin has been proposed. An executable digital twin is a stand-alone and self-contained executable model for a specific set of behaviors in a specific context. It can be leveraged by anyone at any point in lifecycle. To achieve this, a broad toolset of mathematical technologies is required - ranging from model order reduction, calibration to hybrid physics- and data-based models.

In this presentation, we review the concept of executable digital twins, address mathematical key building blocks such as model order reduction, real-time models, state estimation, and co-simulation and detail its power along a few selected use cases.

Scalability of nonlinear problems in contact mechanics and mixed-dimensional coupling - from computational strategies to multigrid solvers

Alexander Popp **PL**

University of the Bundeswehr Munich, Germany

The numerical simulation of nonlinear problems in contact mechanics and mixed-dimensional coupling poses significant challenges for high-performance computing (HPC). The considerable computational effort introduced by the evaluation of discrete contact or mixed-dimensional coupling operators requires an efficient framework that scales well on parallel hardware architectures and is, thus, suitable for the solution of high-fidelity models with potentially many million degrees of freedom. Another unsolved task is the efficient solution of the arising linear systems of equations on parallel computing clusters. In this study, we investigate the scalability of computational strategies and algebraic multigrid (AMG) solvers to address these challenges effectively and ultimately target a faster time-to-solution. Two problem classes of utmost practical relevance serve as prototypes for this endeavor.

First, we investigate the finite element analysis of nonlinear contact problems based on non-matching mortar interface discretizations. Mortar methods enable a variationally consistent imposition of almost arbitrarily complex coupling conditions but come with considerable computational effort for the evaluation of the discrete coupling operators (especially in 3D). We identify bottlenecks in parallel data layout and domain decomposition that hinder a truly efficient evaluation of the mortar operators on modern-day HPC systems and then propose computational strategies to restore optimal parallel communication and scalability. In particular, we suggest a dynamic load balancing strategy in combination with a geometrically motivated reduction of ghosting data. Using increasingly complex 3D examples, we demonstrate strong and weak scalability of the proposed algorithms up to 480 parallel processes. In addition to the computational strategies, we investigate the integration of tailored AMG preconditioners for the resulting saddle point-type linear systems of equations into a then fully scalable simulation pipeline.

Second, we present the mixed-dimensional interaction of slender fiber- or rod-like structures with surrounding solid volumes, thus leading to a 1D-3D approach that we refer to as beam-to-solid coupling. In terms of practical applications, natural and artificial fiber-reinforced materials (e.g., biological tissue, composites) come to mind. Again, not so different from contact problems, the main challenges on the way to a scalable computational framework lie in the efficient and parallelizable evaluation of the underlying mixed-dimensional coupling operators and the design of tailored AMG preconditioners. Here, we will focus on a novel physics-based block preconditioning approach based on AMG that uses multilevel ideas to approximate the block inverses appearing in the system. Eventually, we will assess the performance and the weak scalability of the proposed block preconditioner using large-scale numerical examples.

Isogeometric mortar methods for electromagnetism

Sebastian Schoeps PL

TU Darmstadt, Germany

Isogeometric Analysis was proposed more than ten years ago by Tom Hughes et al. to bridge the gap between computer-aided design and the finite element method. The original method uses Non-Uniform Rational B-Splines (NURBS) for the description of geometry and solution in the context of mechanics. Later, Buffa and Vazquez showed how B-Splines can form a De Rham sequence and thus made the methods interesting for multiphysics simulations including electromagnetism. More recently, mortaring and boundary elements methods have been developed, such that there is a large zoo of isogeometric methods available. This presentation will discuss those methods with the aim to optimize electric machines in the context of e-mobility.

Application of machine learning and computer vision for decision making support during the infrastructure lifecycle

Jelena Ninic **PL**

University of Birmingham, United Kingdom

In the past two decades, the development of cutting-edge soft-computing technologies and their application to engineering problems has demonstrated huge potential to simulate complex non-linear problems. Machine learning and computer vision can play a significant role in supporting decision-making for infrastructure design, construction, and operation in several ways. They are often use for automated design and real-time optimization, virtual control of the construction process, to support real-time monitoring to make informed decisions regarding asset maintenance, repair, or replacement, estimation of the environmental impacts and optimisation of resources or processes to promote sustainability, and so on.

However, the development of robust prediction tools based on Machine Learning (ML) techniques requires the availability of complete, consistent, accurate, and large datasets. The application of ML in structural engineering has been limited because, although real-size experiments provide complete and accurate data, they are time-consuming and expensive. If we look at large infrastructure projects, the available data is often incomplete and associated with uncertainties or is difficult to interpret. Over the past decades, a vast amount of data has been collected about the condition of our structures and stored in asset management systems in reports, however, this data was collected in an unsystematic manner and often presented in a highly subjective way. The average data scientist spends more than 60% of their time on collecting, organizing, and cleaning data instead of the actual analysis. This is why there is an increasing trend of producing synthetic data. While synthetic data offers benefits compared to real-world data (e.g., increased data quality, scalability and interoperability), it is limited mostly due to bias, lack of realism and accuracy, and the inability to represent the response of complex systems.

In this talk, I will discuss the balance of real-word and synthetic data and how to best leverage the strengths of both to maximise the potential of ML to support decision making for design, construction and maintenance of structures and infrastructure. I will reflect on how ML algorithms and their application in structural engineering have evolved over the past decade, their potential and limitations, and the way forward. Finally, I will present several examples of how ML can be used to optimise structural design [1,2], to virtually control the construction process and minimise the impact on the existing environment [3], and to support visual inspection and maintenance of structures, providing a high level of consistency and automation [4].

References

[1] Cabrera, M., Ninic, J. and Tizani, W., 2023.. Eng with Comp, pp.1-19.

[2] Ninic, J., Gamra, A., Ghiassi, B., 2023. Underground Sp.

[3] Ninic, J., et al., 2017. Tun and Underground SpTech, 63, pp.12-28.

[4] Bush, J. et al., 2021. EG-ICE, Berlin, Germany (pp. 421-431).

In vitro, in vivo, in silico: use of computer modeling and simulation in skeletal pathologies and treatment

Liesbet Geris **PL**

1: University of Liege, Belgium; 2: KU Leuven, Belgium

The growing field of in silico medicine is focusing mostly on the two largest classes of medicinal products: medical devices and pharmaceuticals. However, also for advanced therapeutic medicinal products, which essentially combine medical devices with a viable cell or tissue part, the in silico approach has considerable benefits. In this talk an overview will be provided of the budding field of in silico regenerative medicine in general and computational bone tissue engineering (TE) in particular. As basic science advances, one of the major challenges in TE is the translation of the increasing biological knowledge on complex cell and tissue behavior into a predictive and robust engineering process. Mastering this complexity is an essential step towards clinical applications of TE. Computational modeling allows to study the biological complexity in a more integrative and quantitative way. Specifically, computational tools can help in quantifying and optimizing the TE product and process but also in assessing the influence of the in vivo environment on the behavior of the TE product after implantation. Examples will be shown to demonstrate how computational modeling can contribute in all aspects of the TE product development cycle: from providing biological blueprints, over guiding cell culture and scaffold design, to understanding the etiology and optimal treatment strategies for large skeletal defects. Depending on the specific question that needs to be answered the optimal model systems can vary from single scale to multiscale. Furthermore, depending on the available information, model systems can be purely data-driven or more hypothesis-driven in nature. The talk aims to make the case for in silico models receiving proper recognition, besides the in vitro and in vivo work in the TE field.

Mixed-dimensional finite element formulations for beam-to-solid interaction

Ivo Steinbrecher **PL**

Universitaet der Bundeswehr Muenchen, Germany

The interaction between slender fiber- or rod-like components, where one spatial dimension is much larger than the other two, with three-dimensional structures (solids) is an essential mechanism of mechanical systems in numerous fields of science, engineering and bio-mechanics. Examples include reinforced concrete, supported concrete slabs, fiber-reinforced composite materials and the impact of a tennis ball on the string bed of a tennis racket. Applications can also be found in medicine, where stent grafts are a commonly used device for endovascular aneurysm repair, and in many biological systems such as arterial wall tissue with collagen fibers. The different types of dimensionality of the interacting bodies, i.e., slender, almost one-dimensional fibers and general three-dimensional solids, pose a significant challenge for typical numerical simulation methods. The presented focuses on developing novel computational approaches to simulate the interaction between these fiber-like structures and three-dimensional solids. The key idea is to model the slender components as one-dimensional Cosserat continua based on the geometrically exact beam theory, enabling an accurate and efficient description of the fibers. This results in a mixed-dimensional beam-to-solid interaction problem. In a first step positional and rotational coupling between the beam centerline and the underlying solid in line-to-volume problems are addressed. Mortar-type methods, inspired by classical mortar methods from domain decomposition or surface-to-surface interface problems, are used to discretize the coupling constraints. A subsequent penalty regularization eliminates the Lagrange multipliers from the global system of equations, resulting in a robust coupling scheme that avoids locking effects. Furthermore, consistent spatial convergence behavior, well within the envisioned application range, is demonstrated. In a second step, the previously developed algorithms for line-to-volume coupling are extended to to line-to-surface coupling. This introduces the additional complexity of having to account for the surface normal vector in the coupling constraints. Consistent handling of the surface normal vector leads to physically accurate results and guarantees fundamental mechanical properties such as conservation of angular momentum. Finally, a Gauss point-to-segment beam-to-solid surface contact scheme that allows for the modeling of unilateral contact between one-dimensional beams and two-dimensional solid surfaces is presented. The previously mentioned building blocks constitute a novel mixed-dimensional beam-to-solid interaction framework, which is verified by theoretical discussions and numerical examples. Already in the present state, the presented framework is an efficient, robust, and accurate tool for beam-to-solid interaction problems and can become a valuable tool in science and engineering.

Minisymposia

MS 1 ANN and data-driven approaches in material and structural mechanics

Reconstructing orientation maps in MCRpy

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Many data-driven approaches in computational material engineering and mechanics rely on realistic volume elements for conducting numerical simulations. Examples include multiscale simulations based on neural networks or reduced-order models as well as the exploration and optimization of structure-property linkages. This motivates microstructure characterization and reconstruction (MCR). In previous contributions, MCRpy [1] has been introduced as a modular open-source tool for descriptor-based MCR, where any descriptors can be used for characterization and any loss function combining any descriptors can be minimized using any optimizer for reconstruction. A key feature of MCRpy is that differentiable descriptors are available and can be used in conjunction with gradient-based optimizers. This allows the underlying optimization problem to converge several orders of magnitude faster than with the previously used stochastic optimizers [2, 3]. While MCRpy and the gradient-based reconstruction have been presented in previous contributions for microstructures with multiple phases, the present contribution extends these concepts towards orientation maps.

After a brief introduction to MCRpy, the main difficulties of extending gradient- and descriptor-based microstructure reconstruction to orientation maps are discussed. Besides the symmetry of orientation itself after 360°, additional crystal symmetries need to be incorporated and singularities need to be avoided. For this reason, differentiable statistical descriptors are defined in terms of symmetrized harmonic basis functions defined on the 4D unit quaternion hypersphere [4]. Based on a generic combination of descriptors comprising two-point statistics of orientation information and the orientation variation, the optimization problem is defined in the fundamental region of a neo-Eulerian orientation space. These and other measures are motivated and discussed in detail. The capabilities of the method are demonstrated by exemplarily applying it to various microstructures. In this context, it is mentioned that all algorithms are made publicly available in MCRpy and it is demonstrated how to use them. Furthermore, it is shown how to extend MCRpy by defining a new microstructure descriptor in terms of any desired orientation representation or basis function and readily using it for reconstruction without additional implementation effort.

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Achieving desired shapes through laser peen forming: a data-driven process planning approach

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The accurate bending of sheet metal structures is critical in a variety of industrial and scientific contexts, whether it is to modify existing components or achieve specific shapes. Laser peen forming (LPF) is an advanced process for sheet metal applications that involves using mechanical shock waves to deform a specific area to a desired radius of curvature. The degree of deformation achieved through LPF is affected by various experimental factors such as laser energy, the number of peening sequences, and specimen thickness. Therefore, it is important to understand the complex dependencies and select the appropriate LPF process parameters for forming or correction purposes. This study aims to develop a data-driven approach to predict the deformation obtained from LPF for different process parameters. The experimental data is used to train, validate, and test an artificial neural network (ANN). The trained ANN successfully predicted the deformation obtained from LPF. An innovative process planning approach is developed to demonstrate the usability of ANN predictions in achieving the desired deformation in a treated area. The effectiveness of this approach is demonstrated on three benchmark cases involving thin Ti-6Al-4V sheets: deformation in one direction, bi-directional deformation, and modification of an existing deformation in pre-bent specimens via LPF.

Comparison of model-free and model-based data-driven methods in computational mechanics

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In the context of homogenization approaches, data-driven methods entail advantages due to the ability to capture complex behaviour without the assumption of a specific material model. Constitutive model based data-driven methods approximating the constitutive relations by training artificial neural networks and the method of constitutive model free data-driven computational mechanics, directly incorporating stress-strain data in the analysis, are distinguished. Neural network based constitutive descriptions are one of the most widely used data-driven approaches in computational mechanics. In contrast to this, the method of distance minimizing data-driven computational mechanics enables to bypass the material modelling step entirely by iteratively obtaining a physically consistent solution, which is close to the material behaviour represented by the data. A generalization of this method providing increased robustness with respect to outliers in the underlying data set is the maximum entropy data-driven solver. Additionally, a tensor voting enhancement based on incorporating locally linear tangent spaces enables to interpolate in regions of sparse sampling.

In this contribution, a comparison of artificial neural networks and data-driven computational mechanics is carried out based on nonlinear elasticity. General differences between machine learning, distance minimizing as well as entropy maximizing based data-driven methods concerning pre-processing, required computational effort and solution procedure are pointed out. In order to demonstrate the capabilities of the proposed methods, numerical examples with synthetically created datasets obtained by numerical material tests are executed.

Discrete data-adaptive approximation of hyperelastic energy functions

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The prevailing paradigm to model the behavior of rubber-like materials is hyperelasticity. However, phenomenological constitutive modeling is prone to uncertainty and results in loss of information as data coming from experiments are not used directly in calculations. Aside, selecting an appropriate strain energy function for the problem under consideration is left to the engineer and is often based on experience.

Data-driven approaches are a promising alternative to constitutive modeling. We present a new data-adaptive approach to model hyperelastic rubber-like materials at finite strains. Our proposed modeling procedure combines the advantages of phenomenological hyperelasticity with the data-driven paradigm of directly including experimental data in calculations. Import constraints, such as thermodynamic consistency, material objectivity and frame indifference and material symmetry are satisfied a priori. In essence, we suggest formulating a finite-element-like approximation of the strain energy function as a sum of basis functions multiplied by parameters. The basis functions are expanded over the space of invariants which is, in the most generic form, formed by the principal invariants of the right Cauchy-Green tensor. Support points are distributed in the space of invariants, which are the points at which the parameters are defined. In other words, the parameters are the values of the discrete strain energy function at the support points. We consider linear Lagrangian polynomials as basis functions which boils down to (bi)linear interpolation of the parameters. The parameters are determined based on measured full-field displacements, e.g. obtained from Digital-Image-Correlation, and reaction forces by solving a non-linear optimization problem. Within this optimization problem, the 2-norm of the residual vector, which is the difference between measured and computed displacements and reaction forces, is minimized by altering the parameters. The proposed discrete approximation to the strain energy function is flexible enough to discover any admissible form of strain energy function and the fact that our approach does not rely on measured stresses is an advantage over many data-driven approaches presented to date.

We verify our approach and show that computation times are similar compared to those of phenomenological models. By numerical examples, we illustrate that only a moderate number of parameters is required to approximate well-known smooth strain energy functions sufficiently well and demonstrate the ability of our approach to re-identify an extended number of parameters. We also show the robustness of our approach against noisy experimental data.

Physics-Informed Neural Networks (PINNs) for solving inverse problems: constitutive model calibration

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Ensuring the safe and reliable operation of critical load-bearing components requires maintaining their mechanical integrity. Constitutive material models play a crucial role in analyzing mechanical integrity, and their accuracy is essential for assessing the structural integrity of load-bearing components. Notably, mechanical integrity assessments of high temperature components require constitutive models representing the highly nonlinear deformation response of alloys under various loading scenarios and across a wide temperature range. The Chaboche viscoplastic model is among the most well-known constitutive models for representing the isotropic-kinematic hardening behavior of materials. This model employs a set of differential equations to define the viscoplastic strain rate tensor as a function of the stress tensor and several scalar and tensorial internal variables. Calibrating this model for different temperature and loading conditions however requires using experimental data from various mechanical tests and determining a large number of model parameters, which is typically achieved by performing a computationally expensive inverse analysis. To address this computational challenge, we propose a new method that leverages scientific machine learning to accelerate solving the inverse problem. Specifically, we use the Physics Informed Neural Networks (PINNs) framework to incorporate the Chaboche model formulation into neural networks. In this contribution, we illustrate the framework in application to Hastelloy X, by calibrating and determining >30 model parameters based on observations from various cyclic tests at different strain rates in the temperature range of 22-1000°C.

Hamiltonian Neural Network enhanced Markov-Chain Monte Carlo methods for subset simulations

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The crude Monte Carlo method delivers an unbiased estimate of the probability of failure. However, the accuracy of the approach, i.e., the variance of the estimate, depends on the number of evaluated samples. This number must be very large for estimations of a low probability of failure. If the evaluation of each sample is computationally expensive, the crude Monte Carlo simulation strategy is impracticable. To this end, subset simulations are used to reduce the required number of evaluations. Subset simulations require a Markov Chain Monte Carlo sampler, e.g., the random walk Metropolis-Hastings algorithm [1]. The algorithm, however, struggles with sampling in low-probability regions, especially if they are narrow. Therefore, advanced Markov Chain Monte Carlo simulations are preferred. In particular, the Hamiltonian Monte Carlo method explores the target distribution space rapidly. Driven by Hamiltonian dynamics, this sampler provides a non-random walk through the target distribution [2]. The incorporation of subset simulation and Hamiltonian Monte Carlo methods has shown promising results for reliability analysis [3]. However, gradient evaluations in the Hamiltonian Monte Carlo method are computationally expensive, especially when dealing with high-dimensional problems and evaluating long trajectories. Integrating Hamiltonian Neural Networks in Hamiltonian Monte Carlo simulations significantly speeds up the sampling [4]. The extension to latent Hamiltonian neural networks improves the expressivity by adding neurons to the last layer. Furthermore, the enhancement of the No U-Turns Sampler to the Hamiltonian Monte Carlo results in the efficient proposal of the following states [5]. During the exploration of low-probability regions, an online error monitoring calls the standard NUTS sampler if the latent Hamiltonian Neural Network estimates are inaccurate. Based on this recent enhancement, we provide an efficient sampling strategy for subset simulations using latent Hamiltonian neural networks to replace the gradient calculation and speed up the Hamiltonian Monte Carlo simulation.

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Viscoelastic Constitutive Artificial Neural Networks (vCANNs) – a framework for data-driven anisotropic nonlinear finite viscoelasticity

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Finite linear viscoelastic (FLV) or quasi-linear viscoelastic (QLV) models are commonly used to model the constitutive behavior of polymeric materials. However, these models are limited in their ability to accurately represent the nonlinear viscoelastic behavior of materials, particularly in capturing their strain-dependent viscous behavior. To address this issue, we have developed viscoelastic Constitutive Artificial Neural Networks (vCANNs), a novel physics-informed machine learning framework. vCANNs rely on the concept of generalized Maxwell models with nonlinear strain (rate)-dependent properties represented by neural networks. With their flexibility, vCANNs can automatically identify accurate and sparse constitutive models for a wide range of materials. To test the effectiveness of vCANNs, we trained them using stress-strain data from various synthetic and biological materials under different loading conditions, e.g., relaxation tests, cyclic tension-compression tests, and blast loads. The results show that vCANNs can learn to accurately and efficiently represent the behavior of these materials without human guidance.

Advancements in multiscale ML-based constitutive modeling of history-dependent materials

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Many materials exhibit history-dependency in their response. This is evident in the inelastic response of solid materials or in the hysteretic retention curve of multiphase porous materials. Within multiscale simulation of history-dependent materials, the underlying work focuses on testing and comparing different supervised machine learning (ML) approaches to generate suitable constitutive models. This includes the application of recurrent neural networks (RNN), the application of 1D convolutional neural network (1D CNN), and the application of the eXtreme Gradient Boosting (XGBoost) library.

The database used in the supervised learning relies on lower scale two-phase lattice Boltzmann simulations, applied to deformable and anisotropic representative volume elements (RVEs) of the porous materials as presented in [1,2]. In the training, the inputs will include the capillary pressure and its history in addition to the porosity, whereas the output will include the degree of saturation. The comparison among the different ML approaches will include the accuracy in predicting the correct saturation degree and the efficiency concerning the training.

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Locking in physics informed neural network solutions of structural mechanics problems

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Artificial intelligence (AI) applications have recently gained widespread attention due to their capabilities in the domains of speech and image recognition as well as natural language processing. This has drawn research attention towards AI and artificial neural networks (ANNs) in particular within numerous branches of applied mathematics and computational mechanics. The challenge of generating extensive training data for supervised learning of ANNs can be addressed by incorporating laws of physics into ANNs. Most of so-called physics informed neural network (PINN) [1] frameworks for structural mechanics applications incorporate the partial differential equations (PDEs) governing a specific problem within the loss function in the form of energy methods [2] or collocation methods [3].

Many structural mechanics problems are governed by stiff PDEs resulting in locking effects which have already been recognized in the early days of finite element analysis. Locking effects are present for all known discretization schemes, not only for finite elements, independent of the polynomial order or smoothness of the shape functions. This applies to both Galerkin-type solution methods and also collocation methods based on the Euler-Lagrange equations of the specific boundary value problem [4].

In this contribution, we examine the impact of stiff PDEs or locking effects on the accuracy and efficiency of PINN-based numerical solutions of problems in structural mechanics. First investigations on the use of PINNs for solving shear deformable beam and plate problems are presented. Different types of beam and plate formulations, as well as different types of collocation-based loss functions are evaluated and compared with respect to accuracy and efficiency.

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Data-driven discovery of governing equations in Continuum Dislocation Dynamics

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Crystal plasticity is the result of the motion of line like crystal defects, the dislocations. While many traits of crystal plasticity may be described by phenomenological models, the description of the well-known patterning of dislocations as well as the phenomenon of single crystal work-hardening caused by dislocation multiplication during plastic deformation, ask for continuum models rooted more directly in the collective behavior of dislocations. A promising homogenization approach in this realm is the so-called Continuum Dislocation Dynamics (CDD) framework, which is based on conservation laws for tensorial dislocation density measures. In other words, the CDD theory can be considered as a continuum representation of dislocation networks through a hierarchy of tensorial dislocation variables. [1]

In this work, we derive nonlinear expressions for source terms as required in CDD for modeling work-hardening, which is arguably the most salient feature of metal-plasticity. [2] For that purpose we use modern data-driven discovery methods, like the Sparse Identification of Nonlinear Dynamics (SINDy), to describe the highly nonlinear dynamics of dislocation multiplication. The SINDy algorithm is capable of identifying the few predominant terms in the corresponding governing equations based on a model library of predefined, possibly high-dimensional spaces of nonlinear functions using sparse regression techniques. [3]

The SINDy algorithm is applied on a large database of Discrete Dislocation Dynamics (DDD) simulations of the plastic deformation of FCC single crystalline copper under constant strain rate in 120 different loading directions with neglected cross-slip. The extraction of the underlying data of dynamic CDD tensor variables, consisting of density, curvature and velocity tensors of n-th order, from the DDD data is performed by a recently developed algorithm.

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A novel approach to compressible hyperelastic material modeling using physics-augmented neural networks

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The long-standing challenge of simultaneously satisfying all physical requirements for hyperelastic constitutive models, which have been widely debated over the last few decades, could be regarded as "the main open problem of the theory of material behavior"[3]. This is particularly true for neural network (NN)-based constitutive modeling of hyperelastic materials, especially for the compressible case. Therefore, a hyperelastic constitutive model based on physics-augmented neural networks (PANNs) is presented which fulfills all common physical requirements by construction, and in particular, is applicable for compressible material behavior. This model combines established hyperelasticity theory with the latest machine learning advancements, using an input-convex neural network (ICNN) to express the hyperelastic potential. The presented model satisfies common physical requirements, including compatibility with the balance of angular momentum, objectivity, material symmetry, polyconvexity, and thermodynamic consistency [1,2]. To ensure that the model produces physically sensible results, analytical growth terms and normalization terms are used. These terms, which have been developed for both isotropic and transversely isotropic materials, guarantee that the undeformed state is exactly stress-free and has zero energy [1]. The non-negativity of the hyperelastic potential is numerically verified by sampling the space of admissible deformations states. Finally, the applicability of the model is demonstrated through various examples, such as calibrating the model on data generated with analytical potentials and by applying it to finite element (FE) simulations. Its extrapolation capability is compared to models with reduced physical background, showing excellent and physically meaningful predictions with the proposed PANN.

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MS 2 Current trends in modelling and simulation of biological systems: numerics, application and data integration

Modeling neuroblastoma tumour evolution: biomechanical insights and clinical implications

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Neuroblastoma (NB) is the most frequent solid cancer of early childhood. It is a type of cancer that is highly representative of the cancer disease itself, since NB is strongly heterogeneous with very diverse clinical courses that may vary from an indolent disease causing little or no harm and exhibiting spontaneous regression, to an aggressive disease with fatal progression. For these reasons, NB is considered a paradigm of cancer disease and an excellent context of application for the validation of novel developments which have the ambition to be of potential application in a large variety of solid cancers.

NB tumours consist of two main cell populations, neuroblasts and Schwann cells, and the current neuroblastoma classification is based on histological criteria, e. g. the quantity of Schwannian stroma. Neuroblasts and Schwann cells are primary interest herein for contribute directly to the mechanical properties of the tissue through the proliferation and death processes. Extracellular matrix also have a principal role in the cell-microenvironmental cross-talk therefore the tumour can promote to a better stage or keep growing.

We here present a phenomenological model which takes into account as detail as possible to better mimic the real tumour behaviour. Our hypothesis proposes that tumour evolution can be attributed to three distinct processes: growth, shrinkage, and remodelling. The biomechanical model is based on the mass and cellular balance equations coupled with elasticity. The multispecies model simulates the effect of the cellular processes that occur during tumour growth and shrinkage, namely proliferation and death.

The biomechanical finite element model of NB tumour growth starts from imaging data derived mainly from MRI sequences. This data comprises the geometry, the initial cellularity distribution and the tumour vasculature evaluation. At the end of the simulation, the results obtained are validated with a second set of imaging data obtained after treatment.

The study simulates three-month chemotherapy using real patient cases, and presents two distinct outcomes: in one of them, the tumour volume was reduced 20% and in the other one, the volume decreased 90%. One of the patients was classified as low-risk, following the International Neuroblastoma Risk Group (INRG) system, whereas the other was classified as intermediate-risk. Differences appeared in the histology analysis, which reveal one tumour with a higher concentration of tumoural cells, and in the radiomic data obtained after image analysis. The model effectively reproduces these varying outcomes following the application of chemotherapy, facilitating the identification of cases in which the treatment may be effective.

Finite element implementation of the finite deformation-based anisotropic viscoelastic constitutive model of white matter

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Traumatic brain injury (TBI) brought on by a severe head impact in a car accident, a fall, or a sports injury results in internal tissue damage beyond recovery. The human brain mainly has two vital tissues; gray matter and white matter. During accidental impact, forces and torques are imparted in the brain tissues to trigger significant local damage. Although the brain can recover from a TBI, the force necessary to cause permanent brain damage is still not fully understood. One aspect of investigating TBI is to provide a mathematical model and a computational framework to identify the level of injury. Mechanical characterization of the brain tissue is essential to understand brain damage caused by TBI. Since 1960, many studies have been done to understand the brain's mechanical behavior. It is found that brain tissue's behavior is an incompressible, viscoelastic material and anisotropic material. The human brain's finite element (FE) models have been utilized to investigate the risk and mechanisms of traumatic brain injuries. Many human brain FE models have been developed. Many different constitutive models have been used for different parts of the human head. Still, there is scope for improvement in constitutive modeling and its finite element implementation. In this work, we present an anisotropic viscoelastic constitutive model and essential equations for finite element simulations. We implemented the constitutive model by ABAQUS UMAT for doing finite element simulations of the human head FE-model for real-life loading cases. Our uniaxial and cyclic loading simulation using UMAT agree with experimental and MATLAB results.

Effects of hemodynamics in arteries with in-stent restenosis

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The treatment of cardiovascular diseases most often involves coronary stents. Even with drug-eluting stents, implantation can give rise to in-stent restenosis: endothelial denudation and overstretch injuries may result in uncontrolled tissue growth and formation of obstruction to the blood flow. Critical areas where such side effects occur highly depend on the shear stresses and drug distribution inside the artery. For this reason, the analysis of blood flow dynamics in stented arteries is of great interest. The current work is aimed at coupling hemodynamics and tissue growth to include the fluid-structure interaction of pharmacokinetics at the interface between artery and lumen.

Navier Stokes equations and Newtonian constitutive model are used to simulate blood in a stented artery. Wall shear stress (WSS) related quantities are analyzed as indicators of the possible areas of inflammation and thrombosis. Drug elution and deposition on the vessel wall is modeled by means of an advection-diffusion equation and tailored boundary conditions [1]. The convective field is obtained coupling the drug equation to a steady averaged blood flow over three heart beats. Since the healing process and drug elution span a time frame of weeks, a staggered approach is derived to simulate the drug release into the blood stream. Advection-diffusion-reaction equations form the basis of modeling the transport and interaction of species in the vessel wall. The corresponding equations for PDGF, TGF-ß, ECM and SMC can be found in [2]. The drug concentration field is coupled at the interface between the arterial wall and the lumen to account for downstream deposition of the drug. All governing equations for the wall species are coupled to a continuum mechanical description of volumetric growth.

In this work, we test our method on a simplified ring stent geometry with matching interface between the artery wall and the blood domain. We compare the effects of drug coupling and WSS on the endothelium and volumetric growth. All simulations are performed by means of finite element method using FEAP and the in-house code XNS.

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A novel micromorph approach capturing non-local bone remodelling: analysis of bone specimens and loading scenarios

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Bones have the ability to adapt their structure and thus their density to external loads. Cancellous bone, which forms the spongy interior of bones, is a microstructural network of rods. Under- or overloading strengthens or narrows these rods, altering the microstructural pattern. In this adaption process, osteocytes act as mechanosensors, activated by mechanical signals and regulating the mechanical adaptation of bone. That is, they communicate with bone-forming or bone-resorbing cells. Thus, bone remodelling at a particular point is triggered by non-local mechanosensors in its vicinity, i.e. the sensors involved act in a specific sphere of influence and not only locally.

In this work, we present a micromorphic approach that extends the established concept of local bone adaption to account for both the non-locality of bone remodelling and the heterogeneous structure of the material without explicitly resolving it within a two-scale approach. Our approach enables a simple implementation in the open source finite element environment deal.II and avoids the need for laborious neighborhood sampling, as is the case with integral approaches, or for higher continuity requirements, as is the case with higher gradient approaches.

Our approach is phenomenological in nature and refers to nominal bone density to be interpreted as a macroscopic measure of the ratio of bone mass to pore volume in the underlying trabecular microstructure. This way, we account for the heterogeneous microstructure of bone by capturing its effect on nominal bone density, but without actually resolving individual trabeculae. Since bone is a living material, in the continuum approach to bone remodelling we apply the theory of open-system thermodynamics, which assumes that there is a mass source corresponding to the change in nominal density over time. The mass source is equated with a mechanical stimulus, comparing the stored energy to an attractor. The attractor can be interpreted as a biological stimulus that drives remodelling. In the local case, the stored energy is a purely local quantity that depends on the macroscopic deformation. In our novel non-local approach, we now extend this by adding a micromorphic and a scale-bridging component to the stored energy. This allows us to account for non-locality with a characteristic length scale, which acts as a measure for the heterogeneous microstructure and a scale-bridging parameter that penalizes the deviation of the micromorphic from a higher gradient model.

The approach is illustrated in depth and its implications are discussed using benchmark examples. In addition, the modeling approach is discussed using long tubular bones and compared with CT images in health and osteoporosis.

Exploring the mechanical landscape of the human brain

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Human brain tissue shows complex, nonlinear, and time dependent mechanical behavior, and thus presents a significant challenge to those interested in developing accurate constitutive models. Research in our group is focused on better understanding the factors that influence the mechanical response of the tissue. To this end, we combine the mechanical testing of tissue samples from different brain regions under finite deformation in compression, tension and shear with microstructural analyses, continuum mechanics modeling, and finite element simulations. The application of an inverse parameter identification allows us to determine material parameters with a subsequent statistical analysis revealing their regional dependence. Here, we find that the corpus callosum and corona radiata in particular have to be considered as regions with distinct mechanical properties when modeling the whole brain. Furthermore, we analyze the protein content of the tested specimens by enzyme-linked immunosorbent assays and show their correlation with the identified material parameters. These results may motivate and guide the development of microstructurally informed constitutive models that may enable patient-specific predictions.

Personalized computational artery models for coronary stent implantation

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In-stent restenosis is one of the main adverse events after initially successful percutaneous coronary interventions (PCI) with stent implantation. Comprehensive statistical analyses of large clinical datasets identified several independent risk factors for restenosis occurrence, such as patient- or lesion-specific factors, which include small vessel size or the extended length of the stented section. However, it is widely accepted that the local mechanical state within the vessel wall strongly affects vascular growth mechanisms. Nevertheless, these biomechanical factors are currently not integrated into the predictive assessment of lesions at risk. For instance, high intramural stresses and overstretch of healthy vascular tissue during PCI may disturb the natural homeostasis and thus promote excessive tissue growth. Additionally, insufficient stent expansion and incomplete stent apposition reduce the long-term success rate of the procedure. We propose an individualized biomechanical model to study the influence of specific plaque characteristics on the mechanical state of the artery wall during loading conditions experienced in PCI and the final stent placement. In this work, we employ patient-specific artery models based on coronary computed tomography angiography data combined with resolved models of the stent delivery system for physics-informed PCI simulations. We define the system as a computational structural mechanics problem with large deformations and a nonlinear, viscoelastic material formulation for the artery considering the plaque constituents in a heterogeneous manner. The stent structure is resolved and is discretized with reduced-dimensional 1D Cosserat continua with an elastoplastic material formulation. An idealized inflatable balloon model governs the stent expansion. The interaction between balloon catheter and artery is modeled with computational contact mechanics using mortar methods; for the stents, we utilize a beam-to-solid contact approach. All simulations are performed with our in-house multiphysics high-performance code BACI, which uses finite element methods for all problem types considered here. We assess the local stresses and strains within the vessel wall during and after the stent implantation and collate cases with different lesion characteristics. We evaluate the contact between stent struts and endothelium for lesions at risk of incomplete stent apposition. Additionally, we compare the results of our resolved approach to a simplified model, where we model the stent as a pure cylinder with similar mechanical characteristics. In the future, insights from such modeling may inform the clinical assessment of lesions considered for stent implantation.

Exploring biomechanical models with global sensitivity analysis

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Biomechanical models typically contain numerous parameters. Global sensitivity analysis helps identify the most influential and the non-influential parameters, as well as interactions between the parameters.

We show how to apply variance-based global sensitivity analysis to complex biomechanical models. As the method necessitates numerous model evaluations, we utilize Gaussian process metamodels [1] to lessen the computational burden. The approach is illustrated for models of active biomechanical systems by applying it to nanoparticle-mediated drug delivery in a multiphase tumour-growth model [2] and the formation of aneurysms in a model of aortic growth and remodelling [3].

We discover that a small number of full model evaluations suffices to effectively differentiate influential from non-influential parameters, while further evaluations enable the estimation of higher-order interactions. From a biomechanical modeling standpoint, we observe that often a few influential parameters predominantly govern the model output variance. Simultaneously, substantial parameter interactions can exist, emphasizing the necessity for global methods.

Gaussian process-based global sensitivity analysis proves feasible and beneficial for intricate, computationally demanding biomechanical models. Specifically, it can serve as a foundational building block for parameter identification.

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MS 3 Computational modeling and methods for phase-transition problems

Fixed grid methods for phase change - from the Stefan problem to mixture solidification

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Facing phase-change systems ubiquitous in engineering and geophysical applications, we today leverage a range of problem-tailored numerical techniques. Monolithically formulated mathematical models, also referred to as fixed grid techniques [1], consider a single domain containing two or more phases with distinct material parameters, but impose the same governing equations everywhere. It is well known that numerical difficulties arise from the steeply varying material behaviour and the resulting strong non-linearities at the phase-change interface (PCI) [2].

At sufficiently large spatial scales, mixture solidification problems, such as the solidification of alloys or saltwater systems, feature a continuous mushy-layer transition from pure solid to pure liquid. At thermodynamic equilibrium, fixed grid techniques considering just one energy conservation equation for all phases are the de facto standard. While these models theoretically reduce to the classical Stefan problem as the mixture impurity tends to zero, they are often challenging to solve numerically. This is because the implicitly assumed continuity of the mixture PCI, acting as a regularization of the interface non-linearity, is lost in the limit of a sharp Stefan-problem type interface.

In this contribution, we contextualize numerical approaches to single-equation models with applications to solidification of pure substances and mixtures. In particular, we discuss the choice of primary variables in the energy equation, providing a comparative study of enthalpy-based and temperature-based formulations [3]. We examine the two approaches in terms of ease of implementation, accuracy and computational effort and provide a reference simulation based on a level-set method [4]. The methods will be applied both to a solidifying pure substance, where the interface propagation can be interpreted as a Stefan problem, and a binary mixture with a continuous mushy type phase-transition region. Based on our numerical experiments, we will conclude on guidelines to picking the most efficient formulation for the considered problem.

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Unsteady Stefan problem with kinetic interface conditions for rarefied gas deposition

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Phase transition problems in the setting of non-equilibrium thermodynamics appear in various industrial and academical problems. More specifically, sublimation and deposition phenomena involving rarefied gases are important processes in freeze drying in the pharmaceutical area or in the behavior of planetary atmospheres. In these cases, the low-pressure regime is the reason for the rarefaction and consequently for the non-equilibrium behavior.

Modeling non-equilibrium behavior of rarefied gases is challenging as default continuum models can no longer accurately describe them. Instead, the kinetic theory is consulted to derive suitable descriptions.

The Stefan problem is a classical model for phase change problems, originally designed for solid-liquid interactions. We are generalizing this model for solid-gas interaction, so for sublimation and deposition problems. The gas phase is treated rarefied, where the non-equilibrium effects are introduced. A dependency on the well-studied Knudsen and Mach numbers, defined at the phase transition interface, is established. Depending on the level of the rarefaction, the resulting differences from the classical model are significant.

Mass conservation/correction schemes for compressible/incompressible two-phase flow

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Flows with both compressible and (nearly) incompressible species appear in many engineering applications, such as cavitation near propellers or oil-dragging action by blow-by gases in internal combustion engine piston sealing rings[1].

Simulation of these systems can offer insight into the behavior of these systems in the early design stages of products or when investigating a large design space, where building prototypes is more expensive than simulating them. Nevertheless, simulation requires accurate and efficient models for these complex flow phenomena. The level-set method has been used for incompressible two-phase flow with success[2]. It offers intuitive computation of surface curvature based on the signed distance field. For systems where one of the phases is compressible while the other is incompressible, material models have to be used that capture the behavior in both cases. Also, the level-set method does not guarantee mass conservation, requiring special treatment of advection and re-initialization[3]. The models and numerical methods used for this will be presented, as well as results for test and simple application cases.

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On the selective combination of iterative solvers for the implicit time-integration of gradient flow equations with Fourier spectral methods

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Motivated by the vast number of applications of higher-order partial differential equations representing gradient flow like the Cahn-Hilliard equation, the Allen-Cahn equation, the phase-field crystal equation, and the Swift–Hohenberg equation, among others, in this contribution we propose an efficient combination of the Preconditioned Conjugated Gradient (PCG) solver and the recently proposed Iterative Sherman-Morrison Inversion (ISMI) to solve the systems of linear equations that arise during an implicit-time integration of these equations if Fourier-spectral methods are employed for the spatial discretization. PCG is computationally expensive when compared to ISMI, which has a superior convergence, especially during the first few iterations but its computational edge over PCG is lost if too many solver iterations are carried out due to a higher storage demand. Therefore, in this work we propose to selectively combine PCG and ISMI solvers such that the advantages of both solvers are exploited at different stages of the solution scheme which improves the convergence of the residual error of the linear system and thereby the computational efficiency considerably in comparison to standalone versions of the solvers. Some numerical examples are presented in the context of all the aforementioned types of gradient flow in 2D and 3D to demonstrate the benefits of the selective combination in the context of different phase distributions

MS 4 Digital twins and their enabling technologies

Investigation of network architecture and optimizer parameters of physics-informed neural networks

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Physics-Informed Neural Networks (PINNs) have been introduced as a promising method that can combine differential equations and measurement data in the loss function of the neural network [1]. PINNs are a meshless method so they can handle high-dimensional domains. Furthermore, they are a good candidate to solve inverse problems due to the easy integration of data. Based on sensor data, PINNs can be used as a surrogate fast-to-evaluate model in hybrid digital twins of civil engineering structures [2].

One of the main challenges is to find a suitable PINN configuration since the prediction accuracy and model efficiency depend on hyperparameters [3]. Commonly, hyperparameters have been determined by manual adjustment through trial and error. In this contribution, we investigate the network and optimizer parameters of PINNs in various examples aiming for a hyperparameter tuning guideline for computational mechanics problems.

The search space for the network hyperparameters contains the distribution of training points, the number of hidden layers with accompanying neurons, activation functions, and network parameter initializers. On the other hand, the investigated optimizer parameters consist of different optimization algorithms along with their combinations, learning rates and the number of iterations. The main targets of hyperparameter optimization are training performance, loss on collocation and boundary points, and prediction accuracy. Besides a systematic exploration of the search space, we attempt a sensitivity analysis of the optimal PINN configuration in dependence on varying material parameters.

Specific examples include a one-dimensional cantilever beam under a triangular distributed load, a two-dimensional Lam‘e problem and a Hertzian contact problem with the mixed-variable formulation, as well as two- and three-dimensional heat transfer problems and corresponding inverse problems.

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Diverse time scales in multidisciplinary problems - challenges in coupling procedures and software design

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The ever-increasing demand for the integration of high fidelity multidisciplinary simulations in other processes such as optimization and machine learning requires cutting computational costs of each task comprising an analysis, while also ensuring their desired accuracy. Exploiting the inherently different spatial scales that the physical phenomena act on is a proven approach [1] toward achieving this goal. However, such problems often evolve over vastly different time scales as well, but methods taking advantage of this fact [2, 3] are much less mature and lack generalization.

A prime example of diverse spatial and temporal scales is coupling meteorological analyses that have hour-long time steps with local fluid simulations focusing on specific regions, that require temporal resolutions on the scale of seconds, to better capture the influence of local flow effects. Another one is accurately predicting the damage evolution of coupled chemical-mechanical degradation processes, such as the interaction between physical salt attack and dynamic loading on concrete structures.

Partly due to the diversity of the involved phenomena and the wide range of temporal scales, existing multiscale time integration approaches lack a unified structure, greatly limiting their applicability to problems other than what they were designed for. We propose a generic framework for temporal multiscale analyses that incrementally introduce specializations to exact problems in order to help the interchangeability of methods between disciplines. Furthermore, we demonstrate specific applications focusing on meteorology, fluid-structure interaction, and chemical-physical degradation.

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A virtual testbed infrastructure for thermal drilling: application to cryobots

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Thermal drills have become an important tool for the exploration of the cryosphere. In particular, cryobots are employed to access icy environments and retrieve (geo-)physical data, e.g., in Antarctica. In view of future missions to the icy moons of our Solar System, we have to extrapolate the performance of melting probes to extreme conditions that cannot be tested for with experiments on Earth. Thus, digital twins and virtual testbeds will help to develop and improve cryobots for such future missions. In our contribution, we present a testbed that includes environmental data, physics-based forward models for the performance of the cryobots, as well as data-driven approaches based on experimental cryobot data.

First, we need to provide data that can be employed by simulation software. Crysophere measurement data often lack simulation readiness as their (meta)data is inconsistent and incomplete [1]. We developed a tool, named Ice Data Hub, that flexibly stores cryosphere data in a reusable manner and provides interfaces to simulation software. It comes with a GUI to enter, edit, analyze, interpret and export the data. The interface to simulation tools ensures consistent data supply and reproducible preprocessing.

From a modeling perspective, cryobots offer an extremely challenging problem. We have to consider, in fact, a physical object melting its way through a static environment, for which a high-fidelity mathematical model that reflects the probe's dynamic response to the ambient conditions does not exist as of now. Instead, we build upon a model hierarchy of increasing complexity for different simulation purposes. Starting from the energy balance in the microscale melt film, the melting velocity can be derived and integrated into a global trajectory prediction [2]. Alternatively, we can examine the transient ramp-up of the melting process by neglecting equilibrium assumptions. Finally, the evolution of the melt channel around the probe can be modeled by considering the evolving phase-change interface. The aforementioned problems require advanced numerical techniques, such as mesh-update and level-set methods [3].

In this work, we present our simulation models and tools and their integration with the Ice Data Hub. Furthermore, we show test cases of increasing complexity in view of realistic physical scenarios and discuss future extensions.

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Hybrid dgital twin: combining physics-based modelling with data-driven predictions for critical infrastructure

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Digital twins are models that map real physical objects and processes into the digital environment. As the world leans more towards digitalization, digital twins can potentially assist directly in monitoring and protecting critical infrastructure (e.g., bridges), where digital twins can have an essential role in structural health monitoring (SHM) [1]. Hybrid digital twins (HDTs) combine physics-based simulations (virtual twin) with data-based analysis (digital twin), providing a simulation tool with predictive capabilities for damage detection, conditional simulations, and trends identification. In this work, we explore hybrid digital twinning of steel-reinforced concrete beams, and analyse it with experimental data from a real-life structure. Our virtual twin is based on finite element methods with a consistent beam-to-solid volume coupling approach [2]. A model for steel-reinforced concrete structures is created using embedded 1D beam finite elements that enable physics-based modeling to capture the interaction between the reinforcement components and the concrete matrix of the investigated structure. Our digital twin employs physics- informed neural networks (PINNs). The PINNs are trained by optimizing the network weights and biases to reduce the residuals of the partial differential equation, boundary, and initial conditions of a given initial boundary value problem. The network is additionally trained with sensor data to simulate reliable digital representations and provide predictions [3]. The digital and virtual twins can be combined in different approaches, including enriching the digital twin training with the physics-based model and using data-based analysis to enhance the virtual twin. The combination methods of the data-based techniques with physics-based modeling and simulation are studied and contrasted. The model predictions are also compared to the results of physical experiments and sensor data to provide real leverage of the benefits of each twin.

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Strategies for improving the performance of Physics-Informed Neural Networks as reduced simulation models for Stirred Tank Reactors

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Stirred Tank Reactors (STRs) play a central role in biotechnological process development and manufacturing. Digital twins of STRs can be used both to minimize the amount of supporting experimental studies required during process design and scale-up, and to deepen the understanding of conditions inside a reactor, where little information is available due to the lack of appropriate measurement techniques. For this purpose, Computational Fluid Dynamics (CFD) tools are already widely used in the industry. However, the high computational cost of high-fidelity simulations, especially in scenarios, where the same model must be solved repeatedly for different parameter values (such as stirring rate), motivates the construction of less computationally intensive Reduced Order Models (ROMs) to approximate solutions. Physics-Informed Neural Networks (PINNs), originally proposed by Raissi et al. [1], are a promising candidate for ROMs in engineering problems, as they allow to simultaneously exploit both the available data and the knowledge of the underlying physics of the problem by embedding the governing equations in the loss function of the neural network.

This use case represents a particular challenge for PINNs due to the geometric complexity of the computational domain and the large variety of phenomena involved in the process (e.g., turbulence, mass transfer).

Building on the investigation of strategies to improve the predictive accuracy of the model, for example by imposing boundary constraints in a post-processing step using an interpolation spline as proposed in [2] or by leveraging additional knowledge of the problem, such as domain decomposition based on the different character of the flow in different parts of the domain, we aim to apply the approaches tested in 2D to more realistic 3D models. The presented methods can be transfered to other complex problems to improve the overall performance of PINNs.

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A system identification approach for high fidelity parameter models of digital twins

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Digital twins of structures have a wide range of useful applications in fields such as structural health monitoring or predictive maintenance. Furthermore, they enable new methods based on the precise digital representation of a building.

During the lifetime of a building, its condition and state changes. This could be due to a planned change of the structure, damages as a result of use, and/or the degradation of materials. One of the crucial factors for the digital twin concept is that those changes must be reflected in the digital model. Therefore, an automated and robust way to calibrate the structural analysis model so that it meets the necessary criteria to be considered a digital twin is of high importance.

To measure how accurate the digital model is, real world measurements are compared with their corresponding simulation results. These simulations are often driven by high fidelity models (typically based on FEM) with a larger dimensional parameter space. This research aims to directly operate in such high dimensional parameter spaces without reducing is complexity – and thus also keeping the potential richness in information to be adjusted. Using such high fidelity parameter models allows for efficient workflows, a better capture of physical phenomena and a better representation of the real structure, even in complex scenarios.

The resulting inverse problem from such high fidelity models is in most cases highly underdetermined. Hence, to solve such ill posed problems efficiently, an approach based on adjoint sensitivity analysis is selected and different stabilization and regularization techniques are applied. The capabilities and limitations of this approach are demonstrated with illustrative examples.

Physics-informed neural networks for enabling digital twins of profile extrusion processes

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By now, simulations have become an essential tool in engineering sciences. Especially in the field of production engineering, many production processes do not easily allow for measurements. Thus, digital twins, e.g., in the form of high-fidelity simulation models, gain increasing interest as they enable insights into the underlying dynamics of the manufacturing process. However, simulating realistic applications with conventional full-order models is often very expensive due to the large number of degrees of freedom.

This motivates the interest in model-order reduction techniques, which approximate full-order models at much lower computational costs by drastically reducing the degrees of freedom. Here, the recent breakthroughs in deep-learning approaches have drawn attention toward data-based strategies for constructing reduced-order models as alternatives to the well-established full-order models. Many deep-learning-based approaches rely on the abundance of data, which is usually scarce in engineering applications. Utilizing the underlying physics additionally for guiding the learning process has become particularly attractive for constructing accurate but fast digital twins.

In our work, we are interested in the plastic manufacturing process of profile extrusion. Precisely, we are interested in modeling the shear-thinning flow of the highly viscous plastics melt inside profile extrusion dies. To construct a digital twin, we utilize Physics-Informed Neural Networks [1]. We will present comparisons with respect to high-fidelity digital twins, i.e., provided through Finite Element simulation results, and elaborate on training heuristics, which proved essential for our application to obtain reduced models with sufficient accuracy.

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MS 5 Multi-scale modelling and computational approaches to continua with micro-structure

Toughening mechanisms of the Bouligand structure from the perspective of peridynamics

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The Bouligand structure comprises twisted parallel fibers arranged in a helical pattern, which enables greater energy dissipation and fracture toughness, mainly through a large crack surface area and crack-bridging phenomenon compared to regular fiber-reinforced composites. Considering the complex nature of this structure, numerical models that accurately capture the propagation of cracks through its twisted fiber arrangement are limited. This is due to the most popular simulating approach, the finite element method (FEM), is based on the classic continuum mechanics that uses spatial differential equations to describe continuous material behaviors. In contrast, Peridynamics is a computational framework that has been developed to overcome the limitations of classical continuum mechanics in describing crack propagation. Unlike FEM, Peridynamics is a non-local continuum theory that utilizes integral equations instead of differential equations in space to simulate material behaviors. This characteristic makes it highly suitable for modeling the complex crack propagation behaviors in the Bouligand structure. In this study, we present a bond-based peridynamics model to accurately describe the fiber-reinforced composites with a small angle mismatch between adjacent layers in Bouligand structures. To investigate the fracture mechanisms of such a structure, we conduct comprehensive numerical simulations, including 3-point bending and low-velocity impact tests, to obtain detailed information on its deformation and failure behavior. This information is difficult to achieve solely through experimental and theoretical studies. Based on our insights into the toughening mechanisms of the Bouligand structure, we propose a novel approach to further enhance the material's fracture toughness by combining the Bouligand structure with other toughening mechanisms. Overall, the current study provides important insights into the fracture behavior of Bouligand structures and presents new avenues for designing advanced materials with superior mechanical properties.

A Finite Element approach based on an efficient scale bridging concept for ferroelectric continua

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Ferroelectric as well as ferromagnetic materials are widely used in smart structures and devices as actuators, sensors etc. Regarding their nonlinear behavior, a variety of models has been established in the past decades. Investigating hysteresis loops or electromechanical/magnetoelectric coupling effects, only simple boundary value problems (BVP) are considered. In [1] a new scale–bridging approach is introduced to investigate the polycrystalline ferroelectric behavior at a macroscopic material point (MMP) without any kind of discretization scheme, the so–called Condensed Method (CM). Besides classical ferroelectrics, other fields of application of the CM have been exploited, e.g. [2, 3, 4]. Since just the behavior at a MMP is represented by the CM, the method itself is unable to solve complex BVP, which is technically disadvantageous if a structure with e.g. notches or cracks shall be investigated.

In this paper, a concept is presented, which integrates the CM into a Finite Element (FE) environment. Considering the constitutive equations of a homogenized MMP in the weak formulation, the FE framework represents the polycrystalline behavior of the whole discretized structure, which finally enables the CM to handle arbitrary BVP. A more sophisticated approach completely decouples the constitutive evolution from the FE discretization, by introducing an independent material grid. Furthermore, energetic consistencies of scale transitions from grain to MMP and MMP to macroscale are investigated. Numerical examples are finally presented in order to verify the approach.

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A computational multiscale approach to account for material interfaces in electrical conductors

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Every material in nature exhibits heterogeneous behaviour at a certain scale. In a system, defects such as pores, grain boundaries, phase boundaries, secondary phases and particles can be the reasons for heterogeneity. The effective behaviour of the materials is significantly influenced by the underlying microstructure. Interfaces, such as grain boundaries, can affect the overall response of the material under consideration. Experimental findings shows that grain boundaries have a critical influence on electrical properties [1] and in order to model the macroscopic behaviour realistically, interfaces at the microscale should be taken into account.

Motivated by the change of effective electrical properties due to interfaces, e.g. microcracks or grain boundaries, a computational multiscale framework for continua with interfaces at the microscale is proposed in this contribution. More specifically speaking, the computational multiscale formulation for electrical conductors [2] is extended to account for interfaces at the microscale. Cohesive-type interfaces are considered at the microscale, such that displacement and electrical potential jumps can be accounted for. The governing equations for the materials with interfaces under mechanical and electical loads are provided. Based on these, a computational multiscale formulation is established. In particular, averaging theorems for kinematic quantities and for their energetic duals are discussed and their consistency with an extended Hill-Mandel condition for suitable boundary conditions is shown. The coupling between the electrical and mechanical subproblem is established by the constitutive equations at the material interface. In order to investigate deformation-induced property changes at the microscale, evolution of interface damage is elaborated.

To show the capabilities of the proposed framework, different representative simulations are selected. In particular, the calculation of effective macroscopic conductivity tensors for given two-dimensional microstructures is discussed and the fully coupled effective electro-mechanical material response due to the damage evolution is presented.

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On the continuum modeling of flexoelectricity in ferroelectric materials

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The technical relevance of small-scale electromechanical systems is rapidly increasing today. For this reason, the flexoelectric effect, which occurs in all dielectrics, is increasingly getting into the focus of research. This size-dependent effect describes the linear coupling between the electric polarization in the material and an occurring strain gradient in, for example, bent cantilever beams. There also exists a converse flexoelectric effect defined as a mechanical stress response under the action of an electric field gradient especially noticeable at sharp electrode tips in microelectromechanical systems (MEMS). In order to make these coupling effects technically usable, suitable models are required to predict the resulting system response.

A continuum-based model approach that takes into account elastic, dielectric, piezoelectric and flexoelectric effects is presented. Different model variants will be discussed and suitable finite element formulations for solving the electromechanical boundary value problem will be presented. A mixed variation formulation is used here in order to reduce the higher continuity requirements due to the occurring gradient fields. When considering ferroelectric materials (e.g. PZT), microstructural domain switching processes must be taken into account in order to be able to predict the behavior realistically. A microscopically motivated material model representing these dissipative processes is introduced and fitted into the flexoelectric continuum approach. The influence of acting strain and electric field gradients on the domain switching processes in ferroelectrics when considering the flexoelectric effect is studied by numerical experiments.

Immersed isogeometric analysis with boundary-conformal quadrature for thermo-elastic microstructure homogenization

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Numerical simulation of complex geometries and microstructures can be costly and time consuming, in particular due to the long process of preparing the geometry for meshing and the meshing process itself [1]. Several methods were proposed to overcome this issue, such as the extended finite element, meshless, Fourier transform and immersed boundary methods. Immersed boundary methods rely on embedding the physical domain into a Cartesian grid of finite elements and resolving the geometry only by adaptive numerical integration schemes. For instance, the isogeometric finite cell method (FCM) exploits the accuracy of higher-order, smooth B-Spline basis functions for the discretization and employs an octree scheme in order to refine the quadrature rule in trimmed elements. FCM has been applied successfully to various problems in solid mechanics, including linear and nonlinear elasticity, elasto-plasticity, and thermo-elasticity [2]. However, FCM typically requires several levels of refinement of the quadrature rule in order to deliver accurate results, which may lead to high computation times, especially for nonlinear, internal variable, and coupled multiphysics problems.

In this work, we adopt a novel algorithm for boundary-conformal quadrature based on a high-order reparameterization of trimmed elements [3] to solve small and large deformation thermo-elastic problems using spline-based immersed isogeometric analysis (IGA) without the need for a body conformal finite element mesh. In particular, the Gauss points on trimmed elements are obtained by a NURBS reparameterization of the physical subdomains of the cut elements of the Cartesian grid. This ensures an accurate integration with a minimal number of quadrature points. Furthermore, using periodic B-Spline discretizations, periodic boundary conditions for homogenization can be automatically fulfilled. Several numerical examples are presented to show the accuracy and efficacy of the boundary-conformal quadrature algorithm.

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Modeling of polycrystalline materials using a two-scale FE-FFT-based simulation approach

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Components used in the aerospace or automotive industries are often exposed to multi-physical loading conditions and thus may simultaneously be subjected to high stresses and strains as well as temperature changes. Therefore, high-strength and high-temperature resistant materials such as metals are commonly used for applications in this field. Since the overall material behavior is directly influenced by the distribution, size and morphology of the individual grains of the underlying polycrystalline microstructure, detailed knowledge of this microstructural behavior is required in order to accurately predict the macroscopic material response. Hence, multi-scale simulation approaches have been developed. Considering a two-scale finite element (FE) and fast Fourier transform (FFT)-based simulation approach [1, 2], the macroscopic and microscopic boundary value problems are first solved individually by assuming scale separation. In this context, the homogeneous macroscale is subdivided into a discrete number of finite elements. The microscopic boundary value problem is attached to each macroscopic integration point and solved using the FFT-based simulation approach. The scale transition is then performed by defining the macroscopic quantities as the average value over the corresponding local fields. This simulation approach is an efficient alternative to the classical FE^2 method for the simulation of periodic unit cells [3]. To illustrate the applicability of our model, we will present several numerical examples.

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On the second-order computational homogenization of fluid-saturated porous media

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In the present contribution, we deal with a second-order computational homogenization of fluid flow in porous materials. Similar to the first-order computational homogenization in [1], the microscopic problem is formulated employing a minimization-type variational formulation at small strains; see also [2]. While a first-order Darcy-Biot-type fluid transport is considered at the microscale [2], the macroscopic problem is characterized by a second-order material response [3]. Hence, the present formulation allows the relaxation of the scale-separation assumption and the incorporation of the macroscopic second-order terms associated with deformation and fluid-flux fields at the microscale. The macro- and microscale boundary value problems are then bridged via an extended form of the Hill-Mandel condition, which results in suitable boundary conditions at the microscale and a set of constraints [4,5]. Finally, we present numerical examples that provide further insights into the presented formulation.

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Aspects on the modeling of mechanical metamaterials via the relaxed micromorphic model

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Metamaterials are attracting growing attention in industry and academia due to their unique mechanical behaviour. However, when the scale separation does not hold, they show size-effects. Generalized continua can model such materials as a homogeneous continuum with capturing the size-effects.

The relaxed micromorphic model [1] describes the kinematics of each material point via a displacement vector and a second-order micro-distortion field. It has demonstrated many advantages over other higher-order continua such as using fewer material parameters and the drastically simplified strain energy compared to the classical micromorphic theory. Moreover, the relaxed micromorphic model operates between two bounds; linear elasticity with the micro and macro elasticity tensors. The strain energy function in the relaxed micromorphic model employs the Curl of the micro-distortion field and therefore H(Curl)-conforming FEM implementation is necessary [2-3].

In our talk, we will present our recent results in identifying the material parameters and boundary conditions in the relaxed micromorphic model [4].

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Phase-field optimization schemes for periodic micro-lattices with anisotropic properties

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Inspired by lattice structures that can be observed in nature, periodic unit cells and their mechanical properties have caused an ever increasing interest in recent years due to the growing performance of additive manufacturing methods. In order to incorporate cells with optimal properties into printed high-performance structures and devices that can respond to given macroscopic stress-strain states in an optimal manner, one has to provide anisotropic properties that can respond to these individual loads.

We discuss the performance of a phase-field approach for optimizing periodic micro-structures based on triply periodic minimal surface problems (TPMS) to obtain unit cells with an optimal homogenized stiffness response in the direction of the maximal principal stress direction. We show that different TPMS-types exhibit fundamental differences in the way they can respond to uni-axial or shear-dominated loads. An essential aspect in optimizing cells is, on the one hand, to maximize the compliance with external loads and, on the other hand, to limit the danger of failure due to local buckling which is achieved by preserving the connectivity of the cell grid.

Further aspects that are discussed include numerical strategies to handle linear systems of such high-resolution optimization problems in an efficient manner as well as strategies to verify the gain of the homogenized stiffness experimentally.

MS 6 Multiphysical modeling of complex material behavior

Variational formulation of coupled chemo-mechanical problems in elastic and dissipative solids

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In the present work, a variational formulation for coupled chemo-mechanical problems in elastic and dissipative solids at infinitesimal strains is outlined. In doing so, it is seen that the gradient of the primary fields additionally enter the energetic and dissipative potential functions, resulting in additional balance equations. The governing balance equations of the coupled problem are derived as Euler equations of the incremental variational principles, formulated in a continuous- and discrete-time setting. Furthermore, the variables governing the inelastic process are locally condensed which yields a reduced global problem that is solved in a discrete-space-time setting. The symmetric structure of the proposed framework with respect to the primary and state variables is an advantage, and this is exploited in the numerical treatment within the finite element paradigm. The framework is applied to Cahn-Hilliard- type diffusion and Allen-Cahn-type phase transformation in elastic and dissipative solids. The applicability of the proposed framework is demonstrated by means of two- and three-dimensional representative numerical simulations.

A phase field model for ferroelectrics with nonlinear kinetics and electro-mechanical coupling

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Phase field modeling has been widely applied to model the evolution of domain patterns in various phase transformation problems. Existing phase-field models for the evolution of domain structures in ferroelectrics are based on an Allen-Cahn-type evolution law. This evolution law successfully captures equilibrium domain structures. However, it fails to capture rate effects due to its assumption of a linear kinetic relation between the thermodynamic driving force acting on a domain wall and the domain wall velocity. To overcome this limitation, we propose a new phase field model for ferroelectrics (Guin and Kochmann, 2022), one that incorporates nonlinearities in the kinetics of domain walls and fully accounts for electro-mechanical coupling. As a multi-phase-field generalization of the model of Alber and Zhu (2013), it is based on the domain volume fraction of each variant as the primary phase field and incorporates the anisotropic dielectric, elastic, and piezoelectric properties of the different variants. This multi-phase field generalization further allows imposing different kinetic relations in different types of domain walls. This new phase field model is validated through a comparison with the target sharp-interface model embedding nonlinear kinetics. With the ability to easily modify these different material properties, we investigate multiphysical effects to the growth of the ferroelectric embryo, and show the open challenge (in common with all ferroelectric phase field models) of the magnitude of the interfacial energy of the regularized domain wall.

A hybrid microphysical – rheological constitutive model of ferroelectrics within the scope of a multiscale modeling approach

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Ferroelectrics exhibit many interesting effects, both linear and nonlinear, which is why these materials are widely used in science and industry. Recently, the nonlinear effects have also been employed in the field of energy harvesting [1, 2, 3], while for a long time only linear effects were exploited. Moreover, nonlinear effects are irreversible and are accompanied by energy dissipation, which generally leads to a temperature rise of the material. For modeling the characteristic nonlinear effects of ferroelectric materials, there are various possibilities, in particular microphysical and, phenomenological models.

For describing mutually coupled dissipative processes in ferroelectrics, in particular ferroelectric domain switching and viscoelasticity, a hybrid micromechanical - rheological constitutive model is developed and embedded in the framework of a multiscale modeling approach. The mathematical theory is consistent against the background of rational thermodynamics and deals with two types of internal variables. The advanced modeling approach is applied to identify novel energy harvesting cycles exploiting dissipative effects, resulting in a major electric work output.

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A finite element framework for the simulation of material degradation in thermo-mechanics

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The solution of multi-field problems and the numerical implementation by means of the finite element method constitute a sophisticated part of the characterisation of complex material behaviour. Particularly the implementation into commercial finite element codes is of major importance for practical and industrial applications. Although the wide range of available finite element codes (e.g. Abaqus) provides the opportunity for multiphysical modelling, those implementations are rather restricted to the solution of two coupled field equations. In [1, 2] an Abaqus UMAT framework was introduced to use the balance of linear momentum and the heat equation for the solution of two arbitrary coupled field equations of Laplace-type. An extension of the framework to the solution of three coupled Laplace equations is presented in this contribution.

A comprehensive implementation framework for such a three-field problem into the finite element software Abaqus is provided. The procedure is derived for a micromorphic approach in thermomechanics. Although the provided framework contributes to a particular three-field problem, it is not limited to a particular application or a specific number of coupled field equations from a conceptual point of view. The solution of the considered system of equations is separated onto two coupled domains and is based on a two-instance formulation.

To assess the framework for a particular constitutive model, a gradient-enhanced damage model in a thermo-mechanical setting is adopted and representative simulation results are discussed on a local and a global level. Since the framework is not limited to the solution of three coupled field equations, the extension to arbitrary multi-field problems is discussed.

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Dynamic thermo-magneto-visco-elastic modeling of magneto-active elastomers at finite-deformations

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Magneto-active elastomers (MAE) are one of many emerging functional materials. Research applications span mechanical, civil, and biomedical engineering as actuators, sensors, vibration absorbers and vibration isolators. MAE consist of a soft elastomeric matrix filled with small, relatively rigid magnetizable inclusions. Set in a magnetic field, the inclusions deform the microstructure and, at the macro-scale, either stiffen by up to three orders of magnitude or bend to large strains.

Most MAE models focus on magneto-mechanical constitutive relations. This contribution showcases other physical phenomena and their coupled interactions. These phenomena include thermo-mechanical coupling and viscous dissipation leading to heat generation within the material. The model is capable of capturing dynamic effects, particularly when MAE are used as vibration absorbers. Formulated for three-dimensional finite deformations, this model handles incompressible material behavior through a Q1P0 finite element framework.

Permanent magnets generated by severe plastic deformation: a micromagnetic study

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The renewable energy supply, the independence of fossil resources, as well as the change in mobility act as a driving force on technological innovation. To meet these challenges of our time, new and particularly powerful highperformance magnets are necessary [1], relying on new earth abundant materials and resource efficient processes. It has been shown that composite materials consisting of ferromagnetic grains separated by paramagnetic interphases can contribute to significant improvements in coercivity, when these interphases decouple the magnetic exchange between the individual grains, compare [2]. Novel processing routes based on severe plastic deformations (SPD) or additive manufacturing (AM) can be an option to tailor such magnetic composites. Here, the micromagnetic theory can be applied to numerically predict the magnetization distributions on fine scales. Due to their flexibility, finite elements are well suited to discretize and analyze strongly heterogeneous microstructures [3]. The evolution of the magnetization vectors is described by the Landau-Lifshitz-Gilbert equation, which requires the numerically challenging preservation of the Euclidean norm of the magnetization vectors, see [4,5]. With the aim to correctly reproduce the behavior of magnetic materials, competing energy contributions are considered within the energy functional, which are also responsible for the formation of magnetic domains. Also, grain boundaries, defect layers and misoriented grains can have a huge impact on the macroscopic hysteresis behavior of magnetic materials. Especially magnets formed by SPD are exposed to the potential stress-induced defects that might outweigh their

production benefits. Hence, micromagnetics analyses are performed to estimate the risks and challenges of these novelties.

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Topology optimization of flexoelectric metamaterials with apparent piezoelectricity

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We develop a theoretical and computational framework to perform topology optimization of the representative volume element (RVE) of flexoelectric metamaterials [2].

The flexoelectric effect is an electromechanical coupling between polarization and strain gradient as well as strain and electric field gradients, present in small (micro-to-nano) scales [1]. It is universal to dielectrics, but, as compared to piezoelectricity, it is more difficult to harness as it requires small scales and field gradients. These drawbacks can be overcome by suitably designing geometrically polarized metamaterials made of a nonpiezoelectric base material but exhibiting apparent piezoelectricity [3].

We solve the governing equations of flexoelectricity on a high-order generalized-periodic Cartesian B-spline approximation space. The geometry is unfitted to the mesh, and described by a periodic level set function. Genetic algorithms are considered for the multi-objective optimization of the RVE topology, where area fraction competes with four fundamental piezoelectric functionalities (stress/strain sensor/actuator). During the optimization process, the RVE topologies are restricted to be fully-connected in a single group of material.

We obtain Pareto fronts and discuss the different material topologies depending on the area fraction and the apparent piezoelectric coefficient being optimized. Overall, we find RVE topologies exhibiting a competitive apparent piezoelectric behavior as compared to reference piezoelectric materials such as quartz and PZT ceramics. This opens the possibility to design a new generation of devices for sensing, actuation and energy harvesting application using a broad class of base materials.

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Modeling the constitutive behavior of Ferromagnetic Shape Memory Alloys (FSMA) using finite deformation framework

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This study explores the relationship between magnetic fields and deformation in Ferromagnetic Shape Memory Alloys (FSMA), which are materials capable of sensing and actuation. These alloys can exhibit high strains of up to 6% when subjected to a magnetic field. To achieve this goal, a finite deformation formulation approach is proposed based on the multiplicative decomposition of the deformation gradient. In addition, a magneto-thermo-mechanical constitutive model for FSMA is discussed, which is based on a specific Helmholtz free energy function. The evolution equations of the internal magnetic and mechanical state variables are determined using a transformation function, and the model parameters are calibrated under different loading conditions. Finally, the model predictions for FSMA are compared against experimental results.

Understanding AM 316L steel microstructure evolution due to postprocess laser scanning: a thermomechanical modelling and in-situ laser-SEM study

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Studying the evolution of alloy polycrystalline microstructures under the action of thermomechanical loads such as those occurring during metal additive manufacturing (AM), quenching, welding, laser rescanning, etc., can help identify the impact of different process parameters on the origin of residual stresses, plastic deformations, the eventual mechanical response. This information can be used to guide the aforementioned processes to design microstructures with a desired response.

To that end, a polycrystal thermo-elasto-viscoplastic finite element (T-EVP-FE) model has been developed. It takes into account the strong coupling between evolving temperatures and stresses under thermomechanical boundary conditions. The constitutive laws of the model include the generalised 3D Hooke's law, a viscoplastic power law that accounts for the shear rate from each slip system, a Voce-type hardening law, and the generalised Fourier law of heat conduction.

Recently, a series of laser scanning experiments have been performed using a novel laser-SEM (scanning electron microscope) experimental setup; this device is a coupling between a continuous wave fibre laser and an environmental SEM. In these experiments, electron backscattered diffraction was performed before and after laser scanning to study the role of laser scanning on an AM 316L stainless steel microstructure. The experiment revealed the formation of misorientation bands, and hence, geometrically necessary dislocations, that vary as a function of the laser scanning velocity. The T-EVP-FE model has been applied to simulate these laser scanning experiments.

In this talk, the model will be presented, the microstructure state will be compared with experimental observations and the role of laser scan velocity on the evolution of intergranular residual stresses, plastic deformation, stress concentrations, geometrically necessary dislocation formation, etc. will be discussed.

Chemo-mechanical vacancy diffusion at finite strains using a phase-field model of voids as vacancy phase

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High concentrations of vacancies in crystals may be the result of large plastic deformations or irradiation. Void formation and subsequent growth are well-known to be involved in swelling of irradiated materials and seem to play an important role for the nucleation and evolution of porosity in the early stages of ductile failure as recent experiments suggest [1]. Vacancy diffusion and void formation have been modelled using spatially resolved approaches like the phase-field method. Taking into account that vacancies induce an eigenstrain field, which emerges from the relaxation of the surrounding crystal lattice if a single atom is removed, indicates that the evolution of vacancy concentration needs to be properly coupled to the elastic stress field.

In our recent work [2], we proposed a model for coupling elastically driven vacancy diffusion with a phase-field model of void surfaces, which overcomes the short-comings of former models and closely reproduces the sharp interface solution for small-strain elasticity. This is achieved by making the vacancy eigenstrain a function of the non-conserved order parameter used to distinguish the void and crystal phase. With the recent findings and aiming at being able to numerically analyze the early stages of ductile failure as implied by the mentioned experiments, we present the extension of our model to finite strains. Using a multiplicative split for the deformation gradient, a proper coupling of kinematics and the kinetics of vacancy–void interactions is emphasized. A thermodynamically consistent definition of the energy contributions and the derivation of the resulting driving forces based on the underlying phase-field description are outlined. The model is verified with benchmark problems and the influence of the chemo-mechanical coupling is discussed. The implementation of the governing equations in the multi-physics software tool DAMASK [3] allows a coupling to different plasticity laws, like e.g. continuum dislocation dynamics theory for modelling creep or ductile failure.

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Atomistic simulation of (photo)functionalized materials

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In this contribution, we give an overview of methods and techniques that we apply in our group to elucidate the specific behaviour of functional nano-structures in the condensed phase on a molecular basis. A special focus will be on materials that can be reversibly photoswitched by external light stimulus.

Numerical modeling of photoelasticity

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When molecular photo-switches, such as azobenzene or norbornadiene, are embedded into a sufficiently soft polymer matrix the resulting compound can undergo a mechanical deformation induced by light of a specific wavelength. These photo-sensitive compounds have the potential to be applied as soft actuators without the need for hard wired electronics or a separate energy source. Such characteristics are especially attractive in the design of micro-scale robots but also other applications such as high-speed data transfer or the conversion of photonic energy into a mechanical response holds great promise.

Despite these almost futuristic possibilities, photo-sensitive polymers have not yet experienced a sufficient attention in industrial applications. One important factor to increase the acceptance of this group of soft smart materials is the formulation of a rigorous constitutive modeling approach in combination with numerical simulation methods. Thus, in this contribution we present a photo-mechanical modeling approach solved with the help of a finite element implementation.

MS 8 Numerical simulations of flows in porous media

Towards a simulation of repeated wave-induced liquefaction processes

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MS

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A riverbed is a porous medium consisting of a granular skeleton and the pore fluid, which itself comprises water and air. In quasi-saturated conditions, the degree of water saturation ranges from 85 - 99 %. Hydrodynamic boundary conditions affected by, e.g., ship passage influence the hydro-mechanical state of the riverbed. When the intergranular contact forces disappear due to an increase in (excess) pore water pressure, liquefaction occurs, at this point the soil behaves like a fluid instead of a solid. This can lead for example to sediment movement, destabilization of bank protection measures, washed-out submarine pipelines or damaged coastal structures. Modeling of this process requires strong hydro-mechanical coupling and the possibility to represent large deformations. The FEniCS framework was used to solve the underlying partial differential equations in a Lagrangian setting using the finite element method. In addition to the process description, the underlying material model for the soil particle phase must be able to correctly represent the transition from a solid-like to a fluid-like behavior. To date, no approach available in geotechnical software is able to satisfactorily represent the entire process for all associated phases. First steps towards this direction will be shown coupling FEniCS with MFront, which offers the possibility to implement different material models and to incorporate them into different programs via a generic interface. Through this procedure the use of different software packages and even numerical methods becomes practically feasible. First steps towards the identification of a material model, which can represent the bidirectional phase change during liquefaction, will be shown. Experimental data sets generated in a soil column in combination with an alternating flow apparatus serve as a basis for comparison.

Pore-scale simulation of convective mixing in confined media

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We use numerical simulations to investigate the mixing dynamics of a convection-driven porous media flow. We consider a fully saturated homogenous and isotropic porous medium, in which the flow is driven by density differences induced by the presence of a solute. In particular, the fluid density is a linear function of the solute concentration. The configuration considered is representative of geological applications in which a solute is transported and dissolves as a result of a density-driven flow, such as in carbon sequestration in saline formations or water contamination processes. The mixing mechanism is made complex by the presence of rocks (solid objects), which represent obstacles in the flow and make the solute to further spread, due to the continue change of the fluid path. Making accurate predictions on the dynamics of this time-dependent system is crucial to provide reliable estimates of the evolution of subsurface flows, and in determining the controlling parameters, e.g., the injection rate of a current of carbon dioxide or the spreading of a pollutant in underground formations. To model this process, we consider here an unstable and time-dependent configuration defined as Rayleigh-Taylor instability, where a heavy fluid (saturated with solute) initially sits on top of a lighter one (without solute). The fluids are fully miscible, and the mixing process is characterised by the interplay of diffusion and advection: initially diffusion controls the flow and is responsible for the initial mixing of solute. At a later stage, the action of gravity promotes the formation of instabilities, and efficient fluid mixing takes place over the entire domain. The competition between buoyancy and diffusion is measured by the Rayleigh-Darcy number (Ra), the value of which controls the entire dynamics of the flow. We analyse the time-dependent evolution of this system at high Ra, and we quantify the effect of the Rayleigh-Darcy number on solute transport and mixing. Simulations are performed with a highly parallelized finite difference (FD) code coupled with immersed boundaries method (IBM) to account for the presence of the solid obstacles. We compare the results against experimental measurements in bead packs. The results are analysed at two different flow scales: i) at the Darcy, where the buoyancy-driven plumes control the flow dynamics, and ii) at the pore-scale, where diffusion promotes inter-pore solute mixing. Numerical and experimental measurements are used to design simple physical models to describe the mixing state and the mixing length of the system.

A matrix-free discontinuous Galerkin solver for unsteady Darcy flow in anisotropic porous media

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Flow in porous media can be described by the Darcy model in a wide range of applications from soil mechanics to biomechanics. Many relevant applications manifest large scale problems that require transient simulations and finely resolved discretizations. With currently available algorithmic approaches, this can lead to impractically high computing costs or demand to exclude certain effects. For example, current poroelastic models of the human lungs generally solve the steady-state Darcy equation, leaving transient effects unstudied. To address this matter, we propose a new solver for the unsteady Darcy flow problem in anisotropic porous media with spatially and temporally variable porosity and permeability fields.

We use the discontinuous Galerkin method with L2-conforming tensor-product elements for the spatial discretization, and the BDF method for the temporal discretization of the Darcy flow equations. We solve the resulting coupled pressure-velocity system by matrix-free implementation techniques for operator evaluation in Krylov solvers as well as preconditioners. To ensure fast convergence of the solvers, we identify spectrally equivalent preconditioners based on the so-called block preconditioning technique with approximate inverses of the velocity-velocity block and of the Schur complement of the coupled system. For the velocity-velocity block, we design a matrix-free cellwise inverse mass operator with variable coefficients. To minimize arithmetic work, we exploit the tensor-product structure of shape functions using a technique known as sum-factorization. On the other hand, a hybrid multigrid preconditioner for the Poisson problem with variable coefficients approximates the inverse of the Schur complement. We expect these methods to lay a new foundation for high-performance numerical simulations of general Darcy flow.

All methods and applications are implemented in the open source software projects ExaDG and deal.II.

MS 9 Multi-scale shape optimization problems in continuum mechanics

Optimization of the specimen geometry for one-shot discovery of material models

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We recently proposed an approach for Efficient Unsupervised Constitutive Law Identification and Discovery (EUCLID), which exploits machine learning tools such as sparse regression [1–3], Bayesian learning [4], or neural networks [5] to automatically discover material laws independent of stress data, but solely based on full-field displacement and global force data obtained from mechanical testing. The displacement field can be measured on the surface of a target specimen via digital image correlation (DIC).

An important feature of the approach is that, in principle, the discovery of the material law can be performed in a one-shot fashion, i.e., using only one experiment. However, this capability heavily relies upon the richness of the measured displacement data, i.e., their ability to probe the stress-strain space (where the stresses depend on the constitutive law being sought) to an extent sufficient for an accurate and robust discovery process. The richness of the displacement data is in turn directly governed by the specimen geometry.

In the present study, we aim to optimally design the geometry of the target specimen in order to maximise the richness of the deformation field obtained by the DIC method. We seek to excite various deformation modes (from tension/compression to shear) in a single optimised specimen, to maximise the performance of EUCLID. To this aim, we utilise density-based topology optimisation driven by an objective function deduced from EUCLID itself, which essentially aims at enhancing the identification robustness of material parameters (especially in noisy measurements). In this contribution, we shed light on the objective function, the topology optimisation framework, and the initial results.

Unified shape and topological sensitivity analysis for level-set based topology optimization

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Topology optimization is an effective numerical tool to design high-performance, efficient and economical lightweight structures. In this talk the solution procedure for a two material topology optimization problem constrained by a scalar second order PDE is presented. The approach relies on a numerical topological-shape derivative as a main ingredient for the gradient-based solution algorithm.

We state the optimization problem in the continuous setting and subsequently discretize it. On the continuous level we review the classical shape derivative where the perturbation is realized by the action of a vector field and the classical topological derivative where the perturbation is done by means of sets. In contrast to this, in the presented approach the geometry is represented by the zero level-set of a scalar function. Based on this representation we suggest a topological-shape derivative unifying the concepts of shape derivative and topological derivative. In a next step we consider the discretization of the PDE as well as the level-set function by linear triangular Lagrange finite elements. In this numerical setting we can now consider the perturbation of the level-set function by the perturbation of its nodal values. Based on this we give explicit formulas for the computation of the numerical topological-shape derivative. This derivative information is used in an algorithm to update the level-set function where no distinction between shape changes and topological changes is made. The algorithm is tested in a numerical example, where the shape of two circles with different radii is recovered.

Cavity shape optimization in injection molding to compensate for shrinkage and warpage using Bayesian optimization

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In injection molding, shrinkage and warpage lead to shape deviations of the produced parts with respect to the cavity. Caused by shrinkage and warpage, these deviations occur due to uneven cooling and internal stresses inside the part. One method to mitigate this effect is to adapt the cavity shape to the expected deformation. This deformation can be determined using appropriate simulation models, which then also serve as a basis for determining the optimal cavity shape.

Shape optimization usually requires a sequence of forward simulations, which can be computationally expensive. To reduce this computational cost, we use Gaussian Process Regression (GPR) as a surrogate model. The GPR learns the objective function, which measures the shape difference. This difference is computed by taking the average Euclidean distance of sample points on the surface of the deformed product on the one hand and the desired shape on the other hand. Additionally, GPR has the benefit that it allows to account for uncertainty in the model parameters and thus provides a means to investigate their influence on the optimization result. We present a GPR trained with samples from a finite-element solid-body model. It predicts the deformation of the product after solidification and, together with GPR, allows for efficient cavity shape optimization. The optimization parameters are the position of spline points representing the geometry.

To further improve the learning efficiency, we use Bayesian optimization. This approach selects the next training points by utilizing an acquisition function that balances exploration and exploitation. Here, training points with low function values and high uncertainty are given priority. This achieves the goal of finding the optimal solution with the least number of training points. The Bayesian optimization framework was implemented in Python code.

The material parameters can underlie fluctuations because of different batches or when using recycled material. To account for these uncertainties in the material parameters, a new formulation of the objective function is proposed to find the optimal shape resulting in low shrinkage and warpage as well as low variance with respect to the input parameters.

Damage optimisation in forming processes using Abaqus as FE solver

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One phenomenon to consider in metal forming nowadays is the accumulation of ductile damage during the forming process. Ductile damage, i.e. the nucleation, growth and subsequent accumulation of micro-defects such as voids, is inherently present in any formed part. Therefore, it is advisable to reduce these damage effects and in turn produce parts with reduced damage accumulation and thus higher safety factors. Herein, optimisation is a very useful tool to enhance already established processes with damage minimisation in mind. By defining process dependent parameters as the design variables of the optimisation, improved tool sets can be generated to reduce the ductile damage of the formed part.

An important aspect to consider when dealing with simulation of forming processes is the underlying necessity of contact algorithms. Approaches to handle these discontinuous problems are available in literature, by e.g. utilising sub-gradients, however, their application mainly see academic use. The problems for the proposed optimisation are however very complex in nature and therefore require robust and efficient implementation. Consequently, the commercial finite element software Abaqus is used to simulate the processes and solve the necessary contact problems.

In this submission, a framework defined in Matlab is presented, which utilises Abaqus as the finite element program to solve the stated optimisation problems. The framework is applied to different forming processes, such as rod extrusion and deep drawing-like processes, in order to optimise them with regard to their accumulated damage. Different sets of geometric parameters are defined, which in turn result in optimal design for the work tools of the analysed problems. Due to the nature of the framework, the optimisation is not limited to process optimisation and further examples regarding curve fitting for experimental setups are also presented.

Automated surgery planning for an obstructued nose

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The nasal cavity is one of the most important organs of the human body. Its various functionalities are essential for the well-being of the individual person. It is responsible for the sense of smell, supports degustation, and filters, tempers, and moistens the inhaled air to provide optimal conditions for the lung. Diseases of the nasal cavity like chronic rhinosinusitis, septal deviation, or nasal polyps may lead to restrictions or complete loss of these functionalities. A decreased respiratory capability, the development of irritations and inflammations, and lung diseases can be the consequences.

The shape of the nasal cavity varies from person to person with stronger changes being present in pathological cases. A decent analysis on a per-patient basis is hence crucial to plan for a surgery with a successful outcome. Nowadays diagnostic methods rely on morphological analyses of the shape of the nasal cavity. They employ methods of medical imaging such as computed tomography (CT) or magnetic resonance imaging (MRI), and nasal endoscopy. Such methods, however, do not cover the fluid mechanics of respiration, which are essential to understand the impact of a pathology on the quality of respiration, and to plan for a surgery. Only a meaningful and physics-based diagnosis can help to adequately understand the functional efficiency of the nasal cavity, to quantify the impact of different pathologies on respiration, and to support surgeons in decision making.

Physics-based methods to diagnose pathologies in the human respiratory system have recently evolved to include results of computational fluid dynamics (CFD) simulations. In the current study, a reinforcement learning (RL) algorithm that learns to optimize the nasal cavity shape based on feedback from CFD simulations is developed. The final structure of the airway then functions as the proposed surgery. It is investigated how the algorithm finds the optimal structural modification based on various optimization criteria:

(i) the capability of inhaling and supplying the lung with air, expressed by the pressure difference between the nostrils and the pharynx;

(ii) the functionality of the nose for heating up incoming air, represented by the temperature difference between the nostrils and the pharynx;

(iii) the possibility for a balanced air supply between the left and right nasal passages, realized by equal mass flow rates through both nasal passages;

Furthermore, different types of RL algorithms are employed and their computational efficiency is analyzed. It is the aim to further advance these techniques to include them into clinical pathways, thereby allowing personalized analyses on a per-patient basis.

Shape modes of dynamic structures

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This work aims to gain a deeper understanding of sensitivity information through the use of principal component analysis (PCA). By decomposing sensitivity matrices, it is possible to explore and analyze the underlying relationships between variables and the impact of their changes on the overall structure. The approach for this analysis is discussed in [1]. PCA allows us to analyze the eigenvectors of the covariance matrix, which are known as the principal components. The first principal component is considered the most significant mode of variation as it indicates the direction with the highest variance in the data. Similarly, the second principal component represents the direction with maximum variance, but this time it must be orthogonal to the first principal component. This process continues for the remaining principal components. The work at hand makes use of gradient-based sensitivity analysis [2] for dynamic structures and compares two different methods for shape design: Isogeometric Analysis (IGA) [3] and Finite Element Method (FEM). The main focus is on using direct differentiation, but if analytical gradients are not available, numerical differentiation methods such as complex-step method (CSM) can be used as alternatives. We utilize different types of basis functions, such as Bernstein polynomials, B-Splines, and Non-Uniform Rational B-Splines (NURBS), to describe the shape of the structure. IGA has several advantages over traditional FEM-based approaches. These advantages include the ability to accurately describe geometry using fewer control points, high-order continuity, and increased flexibility due to control point weights. These characteristics have a significant impact on shape sensitivity analysis. IGA is used during the structural optimization process to avoid costly remeshing and design velocity field calculations. It is more efficient and effective than traditional FEM approaches for these tasks. In contrast to static analysis, the response of a structure to time-dependent loads is significantly affected by inertia and damping effects. The necessary computational characteristics for this type of problem are discussed and the full solution algorithm is presented.

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Efficient cavity design for injection molding through spline-based methods

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When molding processes, such as injection molding, are used to produce plastics parts, it can be difficult to achieve the correct product shape. As part of the process, the material must cool down and solidify. Since this can happen in an inhomogeneous way, residual stresses can remain in the material. These lead to warpage, after the part is ejected from the machine.

There are several aspects of the process that could be adjusted to improve the resulting product shape. The focus of this work is on the shape of the mold cavity. If suitable adjustments are made to this cavity, the product shape can be improved although shrinkage and warpage still occur. In order to estimate the effects of certain cavity shape changes, a numerical simulation method for the process is required.

This cavity design problem can then be treated either as a shape optimization problem or as an inverse problem. In the former case, a suitable shape parameterization and objective function need to be found. Both options profit from the use of splines, since this allows the shape to be transferred back to a CAD format. The method of Isogeometric Analysis (IGA) offers a convenient way of using splines as a geometry representation in the Finite Element Method. We will discuss the different design approaches and explain the benefits and challenges involved with the spline representations.

Optimization of fiber-reinforced materials to passively control strain-stress response

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The intricate and nonlinear nature of material behavior, characterized by a progressively changing stress-strain relationship, is a fundamental and indispensable property governing the behavior of numerous mechanical systems. Examples of these mechanical systems include rubber components in automobile suspensions and engine mounts, soft tissues and organs in bio-mechanics and medical engineering, as well as packaging materials such as foam, paper, and plastics. Components used for the construction of these mechanical systems often need to meet specific stiffness requirements which can be influenced by the composition of the employed material, see Steinbrecher et al. [Computational Mechanics, 69 (2022)].

On the macro or micro level, such materials can often be classified as fiber-reinforced materials, i.e., thin and long fibers embedded inside a matrix material. One way to control the stress-strain relationship of fiber-reinforced materials is to alter the geometry of the reinforcements, thus creating passive materials with a highly nonlinear stress-strain response. This can be a viable method for the development of optimized system components or meta-materials.

This method can be explored with a single beam embedded in a softer matrix. If the embedded beam is straight, the stress increase would be approximately linear with increasing strain. Bending the beam inside the matrix will lower the starting stress rate. The stress rate increases until the encased beam is straight, at which point the stress rate will not increase further. By manipulating the initial geometry of the beam, the evolution of the strain rate can be influenced.

Previously, Reinforcement Learning based shape optimization has been used to optimize structures in the context of fluid dynamics, see Fricke et al. [Advances in Computational Science and Engineering, 1 (2023)]. This approach is different from classical optimization methods, as it trains an agent to solve a specific task inside a defined problem set. While the training is computationally more expensive than a single optimization, the trained agent is able to optimize a problem inside the learned problem set with less effort.

Applying the RL-based shape optimization method to the beam geometry, an agent is trained to identify optimal beam geometries for a set of starting stress rates and ending stress rates.

Gradient-based shape optimization of microstructured geometries

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Through recent advances in modern production techniques, particularly in the field of additive manufacturing, new previously unthinkable geometries have become feasible. This vast realm of new possibilities cannot be adequately addressed by classical methods in engineering, which is why numerical design techniques are becoming more and more valuable. In this context, this work aims to present concepts that exploit the emerging possibilities and facilitate numerical optimization.

The numerical optimization is built on a microstructured grid, where the geometry is constructed by means of functional composition between splines, resulting in a regular pattern of building blocks. Here, a macro-spline defines the outer contour, a micro-geometry sets the individual tiles and a parameter-spline controls the local parametrization of the microstructure, e.g., acting on the thickness or material density in a specific region. This approach opens up a broad design space, where the adaptivity of the resulting microstructure can be easily extended by increasing the number of control variables in the parameters-spline via h- or p-refinement. The geometric representation uses volume splines, on the one hand providing full compatibility with CAD/CAM and on the other hand facilitating the use of Isogeometric Analysis (IGA). To fully utilize the potential of this type of geometry parameterization, gradient-based optimization algorithms are employed in combination with analytical derivatives of the geometry and adjoint methods.

We will present first results in two fields of application, namely passive heat regulation and an elasticity problem. Here, we demonstrate how optimized microstructures can compensate for irregular boundary conditions and how compliance can be minimized using these lattice-like structures for major weight reduction.

This research has been supported by European Union's Horizon 2020 research and innovation program under agreement No. 862025.

Development of 3D printed adaptive structures for lower limb prostheses shafts

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With an aim to fill the gaps in the current 3D-printing technology to digitally fabricate medical assistive devices with significant user benefit, well-being, and availability; we develop a design methodology that enables the optimization of lightweight multi-material lattice structures in order to enhance the design of prostheses and rehabilitation devices. This is done by firstly developing a suitable multi-variable mathematical model for topology optimization of two-scale structures and secondly demonstrating it on an outer shaft of prostheses (lower limb prostheses shaft). We develop a two-scale gradient-based optimization algorithm procedure of multiple design variables that generates functionally graded structures having excellent performance. Our design methodology employs three families of predefined micro-structures that share similar geometric features. Those two additional families thwart the convergence of our gradient-based algorithm to the global minima and we aim at presenting a computational framework that enhances multi-variable optimizations by avoiding the unfavorable local minima.

Integration of numerical homogenization and finite element analysis for production optimization of 3D printed flexible insoles

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Recently, there has been a development of innovative materials that imitate the strong and lightweight properties of natural structures, such as bones, honeycombs and sponges. These materials have a porous microstructure that alternates between solid and void, and are being used in various fields, especially in healthcare, thanks to advanced manufacturing techniques like 3D printing. However, the production time of 3D printed objects can vary depending on factors such as material rigidity, infill pattern, and printing parameters. To address this issue, a computational tool was developed, integrating numerical homogenization and topological optimization in ANSYS Mechanical. The study used computational homogenization to simulate the mechanical properties of the insoles' infill, investigating various infill patterns in terms of mechanical properties and printing performance. The calculated properties were assigned to the insoles' geometries, and different loading scenarios were analysed, considering therapeutic and usage frameworks. Using the results of these structural simulations, several topology optimization analyses were performed with the objective of reducing the frontal part of the insole's compliance while staying within a specified mass threshold. The study aimed to find a distribution of mass that minimized material use and printing time while maintaining a satisfactory structural response during insole insertion into the shoe. Additionally, this computational approach can optimize the material distribution in various orthopaedic devices, making 3D printing production more effective and reducing printing time.

Adjoint sensitivity analysis for manufacturing constraints in shape optimization

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In the typical product development process of an automotive part, multiple disciplinary teams collaborate to converge on a final design. Structural mechanics, design, crashworthiness and manufacturability are relevant disciplines that mutually influence one another. Sheet metal forming operations are the cornerstone of automotive part production, as a significant portion of the individual components of the Body-in-White (BiW) are fabricated through stamping and deep-drawing processes. Manufacturability assurance for sheet metal forming is commonly addressed by engineering experience and heuristic rules based on geometrical constraints. This work explores the idea of formulating analytical manufacturing constraints for stamped and deep-drawn parts and its inclusion into existing multidisciplinary shape optimization workflows to address formability and performance objectives simultaneously.

As discussed by [1], gradient methods based on adjoint sensitivity analysis, together with a filtering technique as Vertex-Morphing are powerful tools for the typical large and very large optimization use cases in the industry. In this contribution, we present the current progress in the formulation of a constraint for shape optimization that accounts for the manufacturing process, discuss the definition of a meaningful objective function and present details regarding the calculation of adjoint-based sensitivities and its combination with Vertex-Morphing. The formulations of the primal and adjoint problems are also presented, based on the simplified Finite Element Analysis for sheet metal forming proposed by [2].

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MS 10 Computational treatment of slender structures allowing for large rotations

The Hellan-Herrmann-Johnson and TDNNS method for nonlinear Koiter and Naghdi shells

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The development of effective and locking free shell elements is intensive topic of research since several decades. Recently, the Hellan-Herrmann-Johnson (HHJ) method for linear Kirchhoff-Love plates has been extended to nonlinear Koiter shells. Therein, the bending moment tensor is introduced as additional unknown to rewrite the fourth order as a second order mixed saddle point problem circumventing the necessity of C1-conforming finite elements. Via hybridization techniques the saddle point translates into a minimization problem again.

The tangential-displacement and normal-normal-stress continuous (TDNNS) method has successfully been applied to linear Reissner-Mindlin plates leading to a shear locking free formulation.

In this talk we present a shear locking free extension of the TDNNS method from linear Reissner-Mindlin plates to nonlinear Naghdi shells by means of a hierarchical approach. Therefore, the HHJ method for Koiter shells is enriched with shearing degrees of freedom, discretized by H(curl)-conforming Nedelec elements. We discuss the small-strain regime leading to the HHJ and TDNNS method for linear Koiter and Naghdi shells. We show how the so-called Regge interpolant can be used in all methods to avoid membrane locking by inserting into the membrane energy term.

Several benchmark examples, implemented in the open-source finite element software NGSolve (www.ngsolve.org), are presented to demonstrate the excellent performance of the proposed shell elements.

The geometrically exact beam with a projection-based discretization for unit quaternions

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In many different fields of engineering beam models play a significant role in the efficient simulation of slender structures. The most important model for large deformations is the so-called geometrically exact beam also often referred to as Simo-Reissner beam. The configuration manifold of the beam model is given by special Euclidian group as it describes the position of the centerline as well as the orientation of the beam's cross-section. The partial differential equations describing the behavior of the beam is usually solved with the help of the Finite Element Method (FEM). So it becomes necessary to discretize the special orthogonal group in a finite element sense.

A finite element discretization of the special orthogonal group is rather difficult as the special orthogonal group is not an abelian, additive group but a matrix group under multiplication. Though there exist parametrizations of the orthogonal group, which have an additive structure, they result in path-dependency. This can be overcome by discretizing the group directly by using so-called directors. The directors can be discretized additively, so in a classical finite element sense. This, however, leads to an increase in the number of degrees of freedom

if Lagrange multipliers are used to ensure the orthonormality of the directors. Further, this formulation does not conserve the structure of the manifold at every point of the discretization. A possible remedy could be a projection method via the polar decomposition, which is very costly in numerical terms.

The use of unit quaternions for the parametrization presents an interesting alternative. Even though unit quaternions have a complex mathematical structure, it can easily be ensured that their unit length is conserved after a finite element discretization by normalizing the discretized quaternions. This still allows for a classical additive discretization technique in a finite element sense.

In the literature, it is often shown that the Isogeometric Analysis (IGA) is advantageous over the classical FEM with Lagrangian elements, especially for dynamic problems. We thus apply the IGA to the quaternion formulation of the geometrically exact beam.

Analysis and design of deployable structures using the redundancy matrix

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For the description of the load-bearing behavior of structures, the degree of statical indeterminacy is a fundamental property that formally describes the number of missing equilibrium equations necessary to calculate the internal forces. The formal definition of the degree of statical indeterminacy as one single number neglects the distribution of statical indeterminacy within the structure. This neglect can lead to situations where a structure, which is kinematic in one direction and statically indeterminate in another direction is denoted as statically determinate. Thus, mechanisms, which are relevant in the field of deployable structures, and possibilities for prestressing are overlooked. The redundancy matrix, first described by Bahndorf (1991), quantifies the distribution of statical indeterminacy in the structure.

The redundancy matrix is an idempotent matrix, meaning that its eigenvalues are either zero or one. Associated with the eigenvalue of one, which occurs exactly in the quantity that matches the degree of statical indeterminacy, the respective eigenvectors span a space of incompatible elongations (von Scheven et al. (2021)). This space matches the description of self-stress states, described by Pellegrino and Calladine (1986). The eigenvectors associated with the zero eigenvalues span a space that includes states where prescribed elongations match the total elongations. In this case, displacements are present without imposing normal forces, even in statically indeterminate structures. The information about states of stress-free displacements and displacement-free stresses can e.g. be used in the decision-making process of actuator placement in adaptive civil structures (Wagner et al. (2018)) and it might also be used in the adaption process of deployable structures (Veuve et al. (2017)) or for maintenance issues like monitoring stresses in certain parts of a structure.

This contribution presents examples of using the redundancy matrix in the design and assessment of civil engineering structures, especially of deployable structures.

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Hierarchic plate and shell formulations in explicit dynamics

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Recently, the concept of hierarchic structural element formulations has been developed in the group of the authors with a focus on shear deformable Reissner-Mindlin shell formulations [1], [2]. Via reparametrization of the kinematic variables, these formulations possess distinct degrees of freedom for transverse shear. One effect of this hierarchic parametrization is that the resulting elements are intrinsically free from transverse shear locking.

However, the hierarchic structure can also be exploited for an intrinsically selective mass scaling, i.e., a scaling down of the high shear frequencies, which limit the critical time step although being of minor importance for the structural response, while keeping the low bending dominated branch of the frequency spectrum unaffected. This stands in contrast to conventional mass scaling for shear deformable elements, where total rotational inertia is scaled and, therefore, also bending frequencies are manipulated.

In linear kinematics, the hierarchic parametrization leads to an additive structure throughout the kinematic equations, i.e., a clear separation between a Kirchhoff-Love type bending part and an additional shear part. For nonlinear shell kinematics, the assumption of only small shear rotations was made to preserve this additive structure [3].

In this contribution, we present recent investigations on intrinsically selective mass scaling with hierarchic isogeometric structural element formulations and discuss the effects of transverse shear parametrization in transient problems. Additionally, we critically discuss the necessity of a fully nonlinear treatment of shear deformation parts as described in [4].

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On dynamic stability analyses of shells and membranes

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In recent years, increased activity in the field of formulations and discretization methods for thin-walled structures can be observed, see [2], [3], [4], among many others. The topic has received a major boost due to the popularity of the isogeometric concept [1], using NURBS or B-splines as shape functions within finite element analyses. Smooth splines are particularly attractive in problems for which the weak form has a variational index of two or larger, for instance, the Kirchhoff-Love shell model. A further, frequently mentioned key feature of isogeometric analysis (IGA) is the use of “exact” geometry from CAD for analysis.

Preliminary studies for pre-buckling analyses of shells show, that isogeometric shell elements may provide superior accuracy compared to standard shell finite elements in detecting both critical load levels and physical buckling patterns, as can be seen in [5]. That is, for the same level of accuracy, isogeometric shell analyses may require significantly less degrees of freedom compared to finite element analyses. In this contribution, we study whether this superior behavior of IGA can also be observed in more complex non-linear static and dynamic stability analyses of shells and membranes. We systematically study the influence of geometry approximation, polynomial degree and smoothness on the accuracy of results.

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On novel selective mass scaling methods for explicit dynamic analyses of thin-walled structures using solid elements

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The critical time step in explicit transient analyses depends on the highest frequency of the discretized system. In case of thin-walled structures discretized by solid or solid-shell elements, the critical time step, which is a key factor for computational efficiency, is limited by the highest frequencies related to thickness stretch of the elements [1].

Selective mass scaling (SMS) concepts aim at scaling down the highest frequencies, while keeping the low frequencies as unaffected as possible. Most established SMS concepts are designed for discretizations composed of solid or solid-shell elements, as can be seen for instance in [1,2]. They are designed such that at least translational inertia is preserved. Accuracy of these SMS concepts can be increased by extending the construction of scaled mass matrices in such a way that, additionally, rotational inertia is preserved. But this increases computational costs in case non-linear analyses including large rotations, since scaled mass matrices are anisotropic and need to be reassembled during simulation. These additional costs do not pay off in most applications.

In this contribution, we present recent investigations on SMS techniques, which are based on a concept from finite element technology, that is the Discrete Strain Gap (DSG) method [3]. We show that these novel SMS concepts naturally preserve both translational and rotational inertia and possess high accuracy. In addition, having non-linear problem classes including large rotations in mind, we show how to develop efficient isotropic DSGSMS concepts which avoid the need for reassembly of scaled mass matrices.

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Formation of wrinkles in a bi-layer system using manifold-valued finite elements

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We model the formation of wrinkles of an elastic substrate coated with a thin film. The elastic substrate is first stretched, then the film is attached to a part of the substrate boundary in the deformed state. Once the the external force is released, wrinkles form due to the stress mismatch between the two materials. The elastic substrate is modeled using a hyperelastic, homogeneous and isotropic material. The film is modeled using a geometrically exact Cosserat shell. The resulting deformation and microrotation (φ, R) are a minimizing pair of the combined energy functional

$$J(\varphi, R) = \int_{Omega} W_{\text{bulk}}(\nabla\varphi) : dV + \int_{\Gamma_c} W_{\text{coss}}(\nabla\varphi_{|\Gamma_c}, R) : dS$$

in the admissible set

$$\mathcal{A} = \Big\{(\varphi, R) \in W^{1,q}(\Omega, \mathbb{R}^3) \times H^1(\Gamma_c, \text{SO}(3)) : \Big| : \varphi \text{ is a deformation function,}$$
$$(\varphi, R) \text{ fullfill the Dirichlet boundary conditions} \Big\}$$

with $q > 3$.

We discretize the problem using Lagrange finite elements for the substrate displacement. For the numerical treatment of the microrotation field, standard Lagrange finite elements cannot be used, as the microrotation field maps to the nonlinear manifold $\text{SO}(3)$. We present a generalization of Lagrange finite elements that is suitable for such manifold-valued functions: geometric finite elements.

The resulting finite element spaces are complete and invariant under isometries of the manifold. The best approximation error depends on the mesh size h. We prove the existence of solutions of the discrete coupled model. We compare two Newton-type methods to solve the resulting discrete problem: a Riemannian trust-region method and a Riemannian proximal Newton method.

Numerical experiments show that we can efficiently reproduce wrinkling patterns of coupled systems. Our approach works as well for more complex scenarios like multi-layer systems or systems involving various stress-free configurations.

Advanced discretization of director fields based on optimization on manifolds: geometric finite elements, locking, element technology and implementation

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We present an efficient, robust, objective, singularity-free, and path independent formulation for director fields based on optimization on manifolds. This approach allows for accurate and efficient computations of director fields that arise in geometrically non-linear structural models such as the Reissner-Mindlin shell model, in material models of Cosserat-type and in micromagnetic simulations. In this contribution, we investigate the influence of interpolation on manifolds on locking as well as the application of element technologies, such as enhanced assumed strains and the discontinuous Galerkin method.

The numerical methods are implemented into the open source code Ikarus (https://ikarus-project.github.io/), which enables rapid algorithm prototyping, even for optimization on manifolds, thus highlighting the user-friendly interface of this software.

The pertinent constraint for director fields requires to retain unit length of the director during deformation, which can be satisfied by interpreting the constraint as a restriction on the design space. By transforming the problem from 'constrained optimization on an unconstrained space' to 'unconstrained optimization on a constrained space', the structure of the problem is retained, and the design space is reduced. The transformation to an unconstrained optimization problem on a manifold requires generalization of concepts, such as the incremental update of design variables, to account for living on a manifold instead of living in a linear vector space.

For the interpolation on nonlinear manifolds, we utilize the ideas on geometric finite elements presented by Sander (2012) and Grohs (2011). The combination of element technologies such as enhanced assumed strains with the optimization on manifolds approach promises an efficient and accurate solution method for director fields. Numerical examples are presented in the context of micromagnetics, Reissner-Mindlin shells and three-dimensional beams to demonstrate the efficiency and accuracy of the approach.

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MS 11 Stratified turbulence

Mixed convective heat transfer across a turbulent flow over a porous wall layer – a numerical study

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Thermal convection is a phenomenon seen in almost all facets of life, ranging from planetary convection to ocean currents and convection inside the earth. The physics of thermal convection complicates when a porous wall layer is present. Flow over urban canopies, forest canopies or flow in underground aquifers are classic examples of such scenarios where thermal buoyancy-driven convection occurs in the presence of turbulent flow over a porous wall layer. The present research work focuses on simulating pressure-driven turbulent flow over a simplified, ordered porous medium consisting of a regular array of cubes. The work further couples it with natural convection arising due to unstable stratification, to provide insight into the momentum and heat transfer characteristics of such a flow scenario. Direct numerical simulations (DNS) have been performed with a finite-difference solver to validate the model for buoyancy-driven convection and the classical Rayleigh-B´enard convection. Further, we extended the solver with an Immersed Boundary Method (IBM) to model the ordered porous medium, which was validated against reference data. The focal point of the present research, analyzing mixed convection over a porous wall layer, brings into the picture a large number of dimensionless control parameters. The bulk Reynolds in the overlying free channel region is fixed at 5500, the Prandtl number at 0.71. We impose an adiabatic boundary condition on the surface of the cubes. We varied the flux Richardson number to cover different flow scenarios between pure shear and purely buoyancy-driven flows. The porous and free regions are expected to show different convective patterns and different critical flux Richardson numbers for the transition to natural convection cells. Further, the interface regime dynamics should provide insight into the heat transfer characteristics, since the heat transfer timescales vary drastically between the porous region and the turbulent flow region.

Turbulent channel flow with stable stratification beyond Oberbeck-Boussinesq assumptions: a direct numerical simulation study

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Stratified turbulent flows abound in environmental and industrial settings. Examples are atmospheric boundary layer flows, the transport of nutrients and organisms and the mixing of heat and salinity in the oceans, fluid flow in heat exchangers, and the transport of reactants and products in chemical reactions. These examples and many others consider stratified wall-bounded turbulence, in which the creation of turbulence by mechanical processes contends with its dissipation due to buoyancy effects. The buoyancy effects alter the structure of the flow, and consequently the dynamics of mass, heat, and momentum transport. As density fluctuations become more severe, the Oberbeck-Boussinesq approximation becomes inaccurate and the resulting dynamics are not correctly predicted. In the current work, we developed and validated a numerical solver for direct numerical simulations (DNS) of turbulent flows featuring strong property variations. More precisely, we solve the Navier-Stokes equations in the limit of vanishing Mach number (so-called low-Mach number limit), with the fluid density given by the ideal gas law, and the dynamic viscosity and thermal conductivity given by Sutherland's law.

Our numerical solver was then used to study stably-stratified turbulent channel flow under non-Oberbeck-Boussinesq conditions. The simulations will be carried out at friction Reynolds number of 395, Prandtl number of 0.71, and shear Richardson number in the O(10), where the friction Reynolds, Prandtl, and friction Richardson numbers are governing parameters defined based on the prescribed pressure drop and properties of the fluid at the reference temperature. Stratification is achieved by imposing constant temperature boundary conditions, with a high upper-to-lower wall temperature ratio (larger than 2), resulting in strong density variations in the flow. We will vary the temperature ratios and adjust gravity to maintain a similar Richardson number between cases, thereby isolating the effects of strong property variations in the flow dynamics. In the presentation, we will analyze the dynamics of heat and momentum transport under strong stratification for these conditions, also in light of DNS data of the same system under the Oberbeck-Boussinesq regime.

Interaction between capillary waves and hydrodynamic turbulence in a two-layer oil-water flow

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We use pseudo-spectral Direct Numerical Simulation (DNS), coupled with a Phase Field Method (PFM), to investigate the turbulent Poiseuille flow of two immiscible liquid layers inside a channel. The two liquid layers, which have the same thickness (h1 = h2 = h), are characterised by the same density but different viscosities, so mimicking a stratified oil-water flow. This setting allows for the interplay between inertial, viscous and surface tension forces to be studied in the absence of gravity. We focus on the role of turbulence in initially deforming the interface and on the subsequent growth of capillary waves. Capillary wave propagation and interaction is studied by means of a spatiotemporal spectral analysis and compared with previous theoretical and experimental results. Wave propagation is found in agreement with the theoretical dispersion relation. At wave scales larger than the turbulent forcing range the observed scaling of the one-dimensional wavenumber spectrum suggests an energy equipartition regime, which is predicted by theory and recently has been observed in experiments with capillary wave turbulence in microgravity. At wave scales directly forced by hydrodynamic turbulence an initially mild slope of the wavenumber spectrum is succeeded by a sharp decay of wave energy at larger wavenumbers, with the transition taking place near the Kolmogorov-Hinze critical scale, where surface tension forces and turbulent inertial forces are balanced.

Water-lubricated channel flow

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We use direct numerical simulation (DNS) to study the problem of drag reduction in a lubricated channel, a flow instance in which two thin layers of a lubricating fluid (e.g. water) are injected in the near-wall region of a plane channel, so to favor the transportation of a primary fluid (e.g. oil). All DNS are run within the constant power input (CPI) approach, which prescribes that the flow-rate is adjusted according to actual pressure gradient so to keep constant the power injected into the flow. A phase-field method (PFM) is used to describe the dynamics of the liquid-liquid interface and when prescribed, also the presence of surfactants/contaminants. As this technique is tailored toward the transport of very viscous fluids like oils, we study the drag reduction performance of the system by keeping fixed the lubricating fluid properties (water) and by considering two different types of oil characterized by different viscosities, 10 and 100 times larger than that of water, respectively. As these systems are also characterized by the presence of contaminants and surfactants – which act by locally reducing the local value of the surface tension – for each type of transported oil, we consider a clean and a surfactant-laden interface. For all the four tested configurations, we unambiguously show that a significant drag reduction (DR) can be achieved. Upon a detailed analysis of the turbulence activity in the two lubricating layers, the interfacial wave dynamics and their interplay, we are able to characterize the effects of surface tension forces, surfactant concentration and viscosity contrast on the drag reduction performance.

Interaction between thermal stratification and turbulence in channel flow

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Transport phenomena in high Reynolds number wall-bounded stratified flows are dominated by the interplay between the turbulence structures generated at the wall and the buoyancy-induced large scale waves populating the channel core. In this study, we want to investigate the flow physics of wall-bounded stratified turbulence at relatively high shear Reynolds number Ret and for mild to moderate stratification level (quantified here by the shear Richardson number varying in the range 0<Rit<300). By increasing stratification, active turbulence is sustained only in the near-wall region, whereas intermittent turbulence, modulated by the presence of non-turbulent wavy structures (Internal Gravity Waves, IGW), is observed at the channel core. In such conditions, the wall-normal transport of momentum and heat is considerably reduced compared to the case of non-stratified turbulence. A careful characterization of the flow-field statistics shows that, despite temperature and wall-normal velocity fluctuations are very large at the channel center, the mean value of their product (buoyancy flux) vanishes for Rit>200. We show that this behavior is due to the presence of a pi/2 phase delay between the temperature and the wall-normal velocity signals: when wall-normal velocity fluctuations are large (in magnitude), temperature fluctuations are almost zero, and viceversa. This constitutes a blockage effect to the wall-normal exchange of energy. In addition, we show that the friction factor scales as a power of the Richardson number (-1/3), and we propose a new scaling for the Nusselt number (as a function of Reynolds and Richardson number). These scaling laws, which seem robust over the explored range of parameters, are expected to help the development of improved models and parametrizations of stratified flows at large Re.

Assessing non-Oberbeck-Boussinesq effects of convection in cryogenic helium

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Rayleigh-Benard convection (RBC) at high Rayleigh (Ra) numbers represents one of the most important model systems to study turbulent convection [1]. Experiments reaching very high Ra, approaching values relevant for convective systems in Nature, like the atmospheric convection, have been performed using various working fluids, prominently with cryogenic helium 4He [2] and sulphur hexafluoride SF6 [3]. The goal of attaining high Ra often comes at the cost of breaking the Oberbeck-Boussinesq (OB) conditions at the phase boundaries or near the critical points of the working fluids. In particular, the recent analysis [4] of RBC experiments performed near the saturated vapor curves (SVC) in 4He and SF6 indicates that the heat transport measurements of the Nusselt number Nu(Ra), which apparently show the transition of RBC to the ultimate Kraichnan regime, are significantly affected by non-OB (NOB) effects, thus keeping the question of experimental observation of the ultimate regime open. The present study investigates the NOB effects which arise due to the temperature dependence of material properties in cryogenic helium experiments of turbulent RBC. The material properties such as specific heat at constant pressure, dynamic viscosity, thermal conductivity, the isobaric expansivity, and the mass density are expanded into power series with respect to temperature up to the quadratic order with coeffcients obtained from the software package HEPAK. A subsequent nonlinear regression that uses deep convolutional networks delivers a dependence of the strength of NOB effects in the pressure-temperature parameter plane. Strength of the NOB effects is evaluated via the deviation of the mean temperature profile $\xi_{NOB} \equiv T_m - T_c$ from the top/bottom-symmetric OB case $\xi_{NOB} = 0$. Training data for the regression task are obtained from 236 individual long-term laboratory measurements at different Rayleigh numbers which span 8 orders of magnitude. The work has been supported by the Czech Science Foundation project No. 21-06012J.

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MS 12 Modeling and simulation of heterogeneous materials: microstructure and properties

Material modelling for efficient finite element simulation of steel quenching

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Heat treatment plays an essential role in the production of cold-work steel parts. While the material properties are adjusted by the heat treatment, side effects like distortion and residual stresses have to be controlled. A good prediction of the heat treatment plays a major role in reducing the necessary grinding time in subsequent finishing operations. Optimising the heat treatment process has the potential to save energy in the furnaces. This presentation discusses the application of simplified material models for the finite element (FE) simulation of quenching. The formation of martensite is covered by a purely temperature dependent Koistinen-Marburger model, whereas the diffusive formation of Bainite is modelled with an incrementally isothermal Johnson-Mehl-Avrami-Kolmogorov relation [1]. Both models are used in rate format and solved monolithically. The thermal-mechanical-microstructural-coupling implemented in the FE-software Abaqus is presented alongside numerical examples.

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Mechanical properties of additively manufactured lattice structures

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In recent years, the application of lattice structures in additive manufacturing (AM) has gained a lot of attention due to their unique properties, such as high surface-to-volume ratio and self-supporting capabilities. They enable the production of complex parts that are difficult or even impossible to manufacture using conventional methods such as casting or machining. However, despite the advantages of 3D printing over conventional manufacturing technologies, its potential is limited by various phenomena such as warpage due to residual stresses and strains or porosity, leading to a lack of knowledge about the mechanical properties of lattice structures and hindering their commercial application.

To address this shortcoming, this study employs Finite Element Analysis (FEA) to examine the influence of residual stress and porosity defects on the mechanical properties of lattice structures, including Young's modulus, yield strength, and Specific Energy Absorption (SEA). The simulation results are validated through experimental data on the compressive behavior of lattice structures produced through Laser Powder Bed Fusion (L-PBF) with varying parameters. The sequentially coupled thermomechanical finite element model utilized in the simulation evaluates the thermal histories and residual stress evolution throughout the entire AM process. The findings of this study provide valuable insights into the mechanical properties of lattice structures, paving the way for their practical applications in diverse fields.

On the numerical analysis of macro- and microscopic residual stresses in 3D

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Current research aims at the targeted introduction of residual stresses into components during their manufacturing process instead of minimizing them, for example, by subsequent heat treatments. Hot bulk forming processes offer a good opportunity to modify residual stresses in a specific way, since the interactions of thermal, mechanical and metallurgical kind can be exploited. In general, such a hot bulk forming process of a steel component can be divided into three steps: First, the component is heated to over 1000C, which leads to a full austenitization of the material and an assumed to be stress-free initial configuration. Subsequently, forming takes place at this high temperature before the component is cooled down to room temperature. This third step results in a diffusion controlled or diffusionless phase transformation on the microscale based on the cooling rate, see [1].

In this contribution, the focus is on the last process step, i.e., cooling. Different cooling media lead to different phase transformations, which in turn lead to different residual stress distributions in the component. Motivated by the definition of residual stresses, which are characterized by the scale they act on, multi-scale finite element simulations of this cooling process are performed. The comparison of two- and three-dimensional boundary value problems shows the importance of the third dimension to represent the temperature development in the component and to predict residual stress distributions well. For this reason, a three-dimensional FE2 calculation is presented, see [2], in which the microscale is determined by a three-dimensional representative volume element. The resulting residual stresses on macro- and microscale are evaluated and discussed.

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Predicting yield stress in a nano-precipitate strengthened Austenitic steel using an ICME approach

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A recent thrust in structural alloys research is the development of advanced Austenitic steels strengthened by nano-scale precipitates. Of the candidate precipitate phases, nanoscale dispersions of the ordered BCC (B2) NiAl phase have been demonstrated to provide significant increases in yield strength, while allowing reasonable ductility despite the intermetallic nature of this phase. The chemical complexity of the alloy involving small sizes of the particles on the order of few nm severely complicates the physically based prediction of macroscale mechanical properties induced by the characteristics of the particles and their ensembles.

Therefore, we use an integrated computational materials engineering (ICME) approach towards materials design with the aim of predicting mechanical properties such as yield strength based on an input material microstructure. Given the small size and high density of precipitates in the current alloy, we develop a coarse-grained approach for predicting a representative critical resolved shear stress (CRSS) inside local volume elements following the percolation idea for flow-stress from Kocks and Mecking [1]. Using this approach, we model realistic nano-precipitate size distributions in large scale Discrete Dislocation Dynamics (DDD) simulations with the aim of predicting macroscale mechanical properties.

This work seeks to fill the gap in modeling plastic deformation phenomena in stainless steels incorporating chemical heterogeneities on the nanoscale and resulting mechanical properties. Informed by atomistic simulations (DFT/MD), discrete microstructural data extracted from atom probe tomography, and meso-scale modeling (DDD) we present a unique coarse-graining approach in predicting material yield strength for materials with nanoprecipitates.

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Investigation of the role of the barrier parameter for the infeasible primal-dual interior point method for single crystal plasticity

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Modeling single crystal plasticity is essential for understanding the behavior of polycrystalline materials such as metals and alloys. The mechanical properties of such materials depend on the microstructure of individual grains and their interaction through grain boundaries. Single crystal plasticity aims to model the behavior of an individual grain based on the microscopic lattice structure. It can be expressed mathematically using the concept of multisurface plasticity. Applying the principle of maximum plastic dissipation leads to an optimization problem where the individual slip systems of the crystal, represented by yield criteria, define the constraints of the optimization problem.

In the framework of rate-independent crystal plasticity models, the set of active slip systems is possibly non-unique, which makes the algorithmic treatment challenging. Typical approaches are either based on an active set search using various regularization techniques [3] or simplifying the problem in such a way that it becomes unique [1]. In computationally extensive simulations, the problem needs to be evaluated multiple times. Therefore, a stable, robust, and efficient algorithm is required to obtain satisfactory results.

Recently, an alternative strategy based on the infeasible primal-dual interior point method (IPDIPM [2] has been presented in [4], which handles the ill-posed problem without perturbation techniques. Through the introduction of slack variables, a stabilization of the conventional active set search approach is reached. The introduction of barrier terms with related barrier parameters continuously penalizes the violation of the feasibility of the intermediate solution. This talk especially focuses on the treatment of the barrier parameter and the related speed of convergence.

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Data-driven modeling of the plastic yield behaviour of nanoporous metals under multiaxial loading

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Nanoporous metals, built out of complex ligament networks, can be produced with an additional level of hierarchy [S. Shi et al., Science 371, 1026-1033, 2021]. The resulting complexity of the structure makes modeling of the mechanical behaviour computationally highly expensive and time consuming. In addition, multiaxial stresses occur in the higher hierarchy ligaments. Therefore, knowledge of the multiaxial material behaviour, including the 6D yield surface, is required. For finite element (FE) modeling, we separate the hierarchical nanoporous structure into the upper and lower level of hierarchy. This allows independent adjustment of structural parameters on both hierarchy levels and therefore an efficient analysis of structure-property-relationships. Furthermore, a promising approach to significantly reduce computational cost is to use surrogate models and FE-beam models to predict the mechanical behaviour of the lower level of hierarchy.

As a first step towards such a model, we studied the elastic behaviour and yield surfaces of idealized diamond and Kelvin beam models, representation of the lower level of hierarchy, using FE simulations. The yield surfaces exhibit pronounced anisotropy, which could not be described properly by models like the Deshpande-Fleck model for isotropic solid foams. For this reason, we used data-driven and hybrid artificial neural networks, as well as data-driven support vector machines and compared them regarding their potential for the prediction of these yield surfaces. All considered methods turned out to be well suited and resulted in relative errors < 4.5. Of the considered methods, support vector machines exhibit the highest generalization and accuracy in 6D stress space and outside the range of the used training data.

Implementation of the trained SVC into Abaqus [A. Hartmaier, Materials 13, 1060, 2022] results in a promising agreement with the mechanical material response of the original FE beam model, provided that a non-associated flow rule is used. Furthermore, the evolution of the yield surface for higher plastic strains during radial loading were included and as such allow an implementation of the hardening behaviour into the UMAT.

A gradient plasticity formulation to model intergranular damage in polycrystals

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The motion of dislocations has been determined to be one of the main mechanisms leading to inelastic deformation in crystalline materials. Their motion is affected by other crystal imperfections, e.g., at grain boundaries their advancement is hindered due to misalignment between the crystals' slip systems. The pile-up that occurs at the boundaries can lead to yielding inside the adjacent grains or intergranular fracture. The damage induced by the latter acts as a precursor to failure at the macroscopic scale. As such, a formulation capable of describing the interaction between the aforementioned crystal imperfections could provide a feasible tool to predict failure of components made from crystalline materials.

To this end, a gradient crystal plasticity formulation which accounts for grain misorientation is enhanced by considering the grain boundary as a cohesive interface and by introducing a damage variable influencing the interaction between adjacent grains. Numerical examples demonstrating the material response based on the proposed formulation are presented and discussed.

Multiscale modeling of thermal conductivity of concrete at elevated temperatures

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Apart from experimentation, computational models are helpful to aid understanding and subsequently predict the damage processes of concrete under fire, considering physical effects such as chemical dehydration or aggregate-matrix mismatch. These temperature-driven multi-physical deterioration processes are mainly influenced by the macroscopic effective thermal conduction because it predominantly governs the macroscopic temperature distribution. To quantify all degradation factors according to the macroscopic effective thermal conductivity separately, a multiscale model for concrete is proposed.

Four scales of observation characterize the concrete, namely hydrates, cement paste, mortar, and concrete. Based on Eshelby-type homogenization techniques, such as Mori-Tanka and Self-Consistent schemes, the effective thermal conductivity of different blended concretes is calculated at elevated temperatures, considering thermally induced chemical porosity increase of hydrates, initial microcrack density, aggregate degradation, and aggregate-matrix bonding via interfacial transition zones (ITZ).

A stoichiometric model based on an Arrhenius equation is used to predict the volume fraction of chemical dehydration products and porosity at the level of hydrates. The porosity increase and initial crack density lowers the thermal conductivity on the cement paste level, which is calculated using the Mori-Tanaka homogenization framework by considering randomly distributed spherical pores and three orthogonal oriented penny-shaped inclusions, respectively embedded in the matrix material. The effective thermal conductivity of mortar and concrete is determined within the same framework using an analytical expression based on the Kapitza resistance, which characterizes the ITZ morphology.

Concretes with different water-to-cement ratios, aggregate types, and cement paste conductivities are analyzed after the validation process in a sensitivity study comparing the influence on the effective thermal conductivities of concrete at elevated temperatures. Furthermore, the influence of the ITZ morphology and initial crack density is studied in detail. Based on the discussed analyses, it is demonstrated that the model predicts the thermal conductivity deterioration of different concretes or cement compositions from 20°C to 850°C with adequate accuracy.

MS 13 Droplets, bubbles and interfaces in turbulent flows

An enstrophy-based interpretation of turbulence-interface interactions in homogenous isotropic interfacial turbulence

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This study presents a new interpretation of the turbulence-interface interactions during the interfacial fragmentation process based on the concept of enstrophy transport. We carried out fully-resolved volume of fluid simulations of the decaying homogeneous isotropic turbulence in the presence of interfacial structures and analyzed the spectral fluxes of enstrophy production/destruction due to different vorticity transport mechanisms. We highlight the scale-dependent nature of the surface tension mechanism in competition with the vortex stretching mechanism that eventually features two characteristic length scales: (i) the length scale where the spectral rate of surface tension changes sign from negative to positive and distinguishes between enstrophy-reducing fragmentation process and enstrophy-releasing coalescence events across the scales. (ii) The length scale where the rate of enstrophy production by the surface tension balances the disruptive mechanism of vortex stretching. This corresponds to a similar length scale where the energy cascade of two-phase turbulence starts to pile up energy at small scales compared to its single-phase similitude. We further connect the latter to the interfacial statistics and reveal that at this length scale, the size distribution of droplets distinctly changes to a sharper slope. The analysis further discloses that decreasing the surface tension coefficient or viscosity as well as increasing the density of the dispersed phase enhances the vortex stretching effect and dilates the spectral range at which the surface tension contribution is negative toward the smaller scales, and thus facilitates the fragmentation. Whereas the higher surface tension coefficient, higher viscosity, or lower density ratio expands the spectral range associated with a positive contribution of surface tension toward the larger scales and suppresses the fragmentation events. This analysis offers a new interpretation of the Hinze scale in turbulence that is essential for the DNS and LES of two-phase flows.

Heat Transfer in drop-laden turbulent flows

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We investigate the heat transfer process in a multiphase turbulent system composed by a swarm of large and deformable drops and a continuous carrier phase. For a fixed shear Reynolds number (300), a constant drops volume fraction (5.4%), and a fixed Weber number (3.0), we perform a campaign of direct numerical simulations (DNS) of turbulence coupled with a phase-field method and the energy equation; the Navier-Stokes equations are used to describe the flow field, while the phase-field method and the energy equation are used to describe the dispersed phase topology and the temperature field, respectively. Considering several Prandtl numbers, (1, 2, 4 and 8), we study the heat transfer process from warm drops to a colder turbulent flow. Using detailed statistics, we first characterize the time evolution of the temperature field in both the dispersed and carrier phase. Then, we develop an analytic model able to accurately reproduce the behaviour of the dispersed and continuous phase temperature. We find that an increase of the Prandtl number, obtained via a decrease of the thermal diffusivity, leads to a slower heat transfer between the dispersed and carrier phase. Finally, we correlate the drop diameters and their average temperatures.

Bubble flows: phase field methods compared

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Most industrial processes involve multiphase turbulent flows. Therefore, understanding the underlying physics is of primary importance for reducing pollutant emissions and also for improving the safety protocols in industry processes. In this regard, numerical simulations provide a valuable tool due to their lower cost compared to experiments. Furthermore, simulations allow us to overcome current instrumentation limits. In this context, the phase-field method is coming to the fore for its ease of implementation and good scalability. However, its most well-known implementations, based on the conservative Cahn-Hilliard equation, have limitations on the density and viscosity ratios preventing us from studying realistic cases. Recently, novel approaches proposed a conservative Allen-Cahn equation which guarantees the solution boundedness. We show the results of a 2D rising bubble in a quiescent fluid at Reynolds 10 where the motion is only due to the density ratio between the carrier and dispersed phase. In particular, two different density ratios are analysed: 0.1, 0.01. We characterize the shrinkage phenomenon by comparing the instantaneous profiles of the phase field with the theoretical profiles, then we quantify the mass loss in each case.

Towards direct numerical simulation of compressible droplet grouping in turbulent flows

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The tendency of initially distant droplets in gas flows to convene and form clusters - known as droplet grouping - is an important phenomenon which affects evaporation rates and combustion dynamics, for example. Despite its relevance to technical applications, this grouping behavior and its governing factors are not yet fully understood, in particular in turbulent, compressible flows. Therefore, related work often focuses on a laminar, monodisperse droplet stream, which consitutes the most fundamental configuration subject to grouping and has been studied analytically, numerically as well as experimentaly.

While those investigations consider incompressible gas flows, this talk examines the grouping behavior in the compressible regime through direct numerical simulation (DNS), using a high-order level-set ghost fluid framework. We address arising challenges such as the mass loss inherent to the level-set method and propose a simple approach to track the individual droplets through the computational domain. In order to gain insights into the grouping mechanics, the impact of the initial droplet alignment, the Reynolds number and other parameters is studied in detail. The results are also compared with reference data from experiments and incompressible DNS to unveil compressibility effects in droplet grouping.

Coherent vortical structures and energy dissipation in wave breaking with energy preserving multiphase solver

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The flow generated by the breaking of free-surface waves in a periodic domain is simulated numerically by means of a gas-liquid multiphase Navier-Stokes solver. The solver relies on the Volume-of-Fluid (VOF) approach, and interface tracking is carried out by using a novel algebraic scheme based on a tailored TVD limiter (Pirozzoli et al., 2019). The solver is proved to be characterized by low numerical dissipation, thanks to the use of the MAC scheme, which guarantees discrete preservation of total kinetic energy in the case of a single

phase. The low artificial dissipation and the potentiality of the algebraic VOF used is analyzed and highlighted through the simulation of the benchmark proposed by Estivalezes et al., 2022, where the ability of algebraic VOF to work for both miscible and immiscible fluids is demonstrated, allowing lower dissipated energy. After, both two- and three-dimensional simulations of wave breaking have been carried out, and the analysis is presented in terms of energy dissipation, air entrainment, bubble fragmentation, statistics and distribution. Particular attention is paid to the analysis of the mechanisms of viscous dissipation. For this purpose, coherent vortical structures (Horiuti and Takagi, 2005), are identified and the different behaviour of vortex sheets and vortex tubes are highlighted, at different Re. The correlation between vortical structures and energy dissipation demonstrates clearly their close link both in the mixing zone and in the pure water domain, where the coherent structures propagate as a consequence of the downward transport. Notably, it is found that the dissipation is primarily connected with vortex sheets, whereas vortex tubes are mainly related to flow intermittency.

MS 14 Mechanics of soft multifunctional materials: experiment, modeling and simulation

On the magnetostrictive and fracture behavior of soft magnetorheological elastomers: influence of magnetic boundary conditions

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Magnetorheological elastomers (MREs) with soft matrices have paved the way for new advancements in the fields of soft robotics and bioengineering. The material response is governed by a complex magneto-mechanical coupling, which necessitates the use of computational tools to guide the design process. However, these computational models typically rely on finite element frameworks that oversimplify and idealize the magnetic source and magnetic boundary conditions (BCs), leading to discrepancies with the actual behavior even at a qualitative level. In this study, we comprehensively examine the impact of magnetic BCs and highlight their significance in the modeling process. We present a magneto-mechanical framework that models the response of soft-magnetic and hard-magnetic MREs under various magnetic fields generated by an idealized magnetic source, a permanent magnet, a coil system, and an electromagnet with two iron poles. Our results demonstrate noteworthy differences in magnetostriction depending on the magnetic source used. Furthermore, we implement a virtual testbed to explore the fracture performance of MREs with remanent magnetic fields. To this end, we prescribe remanent magnetization conditions on rectangular samples, and we add a damage phase-field to model crack propagation. In order to maintain the continuity of the magneto-mechanical fields, the damaged material is designed to exhibit the same behavior as the surrounding air. The results show that remanent magnetization enhances the fracture energy and arrests cracks propagation.

Refs:

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A phase field model for crack propagation in electroactive polymers

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Electroactive polymers are a class of smart materials which change shape when stimulated by an electric field. Typical applications are in the areas of, e.g., robotics, artificial muscles and sensors. For such applications a reliable prediction of properties and performance, including loading and performance limits, is important. The occurrence of damage and fracture has a strong influence on the material behaviour. In this context, this work combines a material model for electroactive polymers with a fracture model.

The behaviour of electroactive polymers is modelled as a quasi-static large strain electro-mechanical material. The model is derived from a potential. The mechanical part of the model is a Neo-Hooke material and the electro-mechanical coupling is described by the relative permittivity. The material parameters are chosen such that the model mimics the behaviour of a soft electroactive polymer. The model is analysed with respect to the physically reasonable response and numerical stability. A phase field model for crack propagation is applied as fracture model. This method describes the crack propagation by means of an additional scalar field, the phase field. This phase field takes values between zero and one, whereby value zero represents undamaged material and value one corresponds to a fully damage state, respectively crack at the particular location. Since the model is used for polymers, the phase field model is adapted to large strains. The electro-mechanically coupled problem is solved within a monolithic scheme. The phase field problem, however, is solved within a staggered algorithm. The crack-propagation turns out to be different for the purely mechanical case as compared to the electro-mechanically coupled case.

The proposed model is implemented in a nonlinear finite element framework. Representative numerical examples are discussed in order to show the applicability of the model.

Surface elasticity in soft solids

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Soft solids such as silicone gels, with bulk shear modulus ranging from 10 to 1000 kPa, often exhibit strongly strain-dependent surface stresses. Moreover, unlike conventional stiffer materials, the effects of surface stress in these materials manifest at length scales of tens of micrometers rather than nanometers. The theoretical framework for modelling such problems envisages a soft hyperelastic bulk on which the infinitesimally thin surface that acts as a 'wrapper', with its own constitutive equation. We will recall the essential features of this theoretical framework and its FE implementation in the first part of this talk.

In the second, we will highlight simple force-twist, torque-twist, and force-extension (force-compression) responses of a soft cylinder held between two inert, rigid plates to demonstrate the role that the parameters in the surface constitutive model play in modulating the overall response of the bulk-surface system.

Finally, we will, through Finite Element simulations, demonstrate the effect of surface elasticity on two problems. The first is a variation of the well-known problem of an axisymmetric liquid capillary bridge between two rigid surfaces, with the liquid replaced by a soft solid. When the associated length scales are small, the shapes of the meniscus of a soft solid capillary with significant surface elasticity exhibits a much richer variety of shapes than a liquid. However, with stretch, the meniscus tends behave like a liquid bridge.

In the second problem, we explore the recent rather counter-intuitive experimental observation that, soft solids, when reinforced with small liquid inclusions, can become stiffer than the matrix material. We perform computational homogenisation on liquid inclusion reinforced soft solids with a view to understand the effect of surface stresses on their overall stiffness and manner in which cracks propagate in them.

Swelling induced deformation of hydrogel

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Hydrogels are three-dimensional networks of polymer chains that are linked together by chemical and physical crosslinks. They are highly swellable, capable of changing chemical energy to mechanical energy and vice versa. They have unique properties such as low elastic moduli and large deformability. The main constituent of hydrogels are the polymer chains that are highly hydrophilic. When immersed in water they absorb water molecules increasing the volume, resulting in swelling. This generally takes place in three steps: one, diffusion of water into the polymer network, two, relaxation of network chains and three, expansion of the polymer network. Normally hydrogels in the fully swollen state are viscoelastic and rubbery, similar to the biological fluids. These properties make them biocompatible. Thus, hydrogels have found applications in biomedical fields, such as making contact lenses, wound dressings, and tissue engineering. They are also used in fluid control and drug delivery systems. In this work, we focus on free swelling of a hydrogel from dry state to fully swollen state. We take the polyacrylamide (PAAm) hydrogel with degree of swelling Q = 42.5. Further, we use this state as the reference state and apply uniaxial load in tension. We assume that swelling is homogeneous. We focus on the non-linear theory of swelling. We plot the stress versus stretch diagram under uniaxial loading conditions. The model is validated with the available experimental results.

Magneto mechanical experiments on soft Magneto Active Polymer

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Magneto Active Polymers (MAPs) are composite material that combines micron-sized magnetic particles with an elastomer matrix. These materials are notable for their softness and ability to become stiffer in response to an external magnetic field. MAP is prepared by mixing micron-sized iron particles with an elastomeric matrix (i.e., PDMS), which is one of the varieties of silicon rubber. Here we present a study on the mechanical characterization of magneto active polymers prepared by mixing iron particles with a Polydimethylsiloxane (PDMS) (Ecoflex polymers) matrix. The stiffness of PDMS depends on the mixing ratio of these two components. Tensile and relaxation tests were conducted to characterize the mechanical properties of MAP. The experimental data obtained from these tests were used to calibrate the model for the material and to determine the elastic and viscoelastic constants. The results of the study showed that the MAP exhibited desirable mechanical properties and that the external magnetic field can control its response. The calibrated model effectively predicted the mechanical behavior of the material under different loading conditions. The findings of this study have significant implications for the development of magneto active polymers for various applications, such as in the field of soft robotics, where the material's mechanical properties play a crucial role in the design and operation of soft robots.

Towards the simulation of multistable microstructures of extremely soft magnetorheological elastomers

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Two decades ago, new experiments accompanied by the modernization of magnetoelastic theory have spawned a great amount of theoretical, numerical but also experimental developments on magnetoelastic composites such as magnetorheological elastomers (MREs). Thanks to extensive research efforts, their coupled magnetoelastic response is well understood nowadays. However, this applies only to MREs and related materials based on sufficiently stiff matrix material. Indeed, as the shear modulus of the matrix material is reduced further and further, magnetoelasticity turns out to be an insufficient theoretical framework at the macroscopic scale as demonstrated in this contribution. Even when neglecting the dissipation in the constituents, one may observe significant dissipation.

In composites based on very soft matrix material that can only store rather small amounts of elastic energy, the magnetic energy may dominate the total energy of the system. Multiple (meta-)stable configurations are the consequence, which render the composite material "magneto-pseudoelastic" even when both the inclusions and the matrix material are practically non-dissipative. While such “magnetodeformal shape-memory” effects can be found in mainly experimental literature, we are not aware of quantitatively predictive simulations in this regard.

In this talk we present ongoing work pushing the limits of finite element and re-meshing technologies in order to render the complicated processes extremely soft MREs accessible by computational means.

Advanced constitutive modelling of polymers for tissue bioprinting applications

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Modern 3D bioprinting techniques aim at reproducing a specific tissue composition by extruding a bioink, which is a cluster of stem cells embedded into a hosting gel, into the desired pattern. If the extruded structure is fed suitable nutrients, cell differentiation and growth is initiated. However, prior to activating these processes, the gel must first be converted into a polymer construct to provide support and preferential directions to the successive cellular growth phase. There are many ways to accomplish this melt-to-solid transition, most notably photo-polymerisation. The irradiation of a light with suitable intensity and wavelength triggers chemical processes that induce the cross-linking between polymer chains within the printed material, in a time-evolving scheme of structure formation. Controlling this process holds great importance, since cellular motility and nutrient diffusion are greatly affected by the disposition and orientation of the polymer network. As it currently stands, the 3D printing process briefly described above is well known, but in many instances it is not yet adequately optimised and the influence of a variety of parameters hinders a large-scale production basis. For example, the intensity and direction of the UV light has no standard protocol yet, so the definition of an optimal disposition of the light sources can prove essential in minimising the polymerisation times, hence tissue formation times as a whole. This work intends to ground the choice of selected polymerisation parameters to a rational basis. To achieve this, the relevant Physics of what happens after the melted bio-ink is deposited has been represented through multi-physics Finite Element simulations, where the kinetics of polymer cross-linking has been coupled with finite deformation formulations. Viscoelastic behaviour during polymerisation has also been accounted for. To deal with the highly non-linear differential equations representing the problem, a parametrised custom Finite Element variational formulation has been implemented.

MS 16 Modeling, simulation and quantification of polymorphic uncertainty in real word engineering problems

Surrogate assisted data-driven multiscale analysis considering polymorphic uncertain material properties

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Composite materials, such as (reinforced) concrete, which are designed by combining different constituents to obtain materials with beneficial properties for specific applications, are involved in many current research topics. The combination of different materials yields heterogeneities. These must be taken into account in the numerical simulation in order to obtain realistic results. Traditionally, the FE2 method based on the concept of numerical homogenization is used to obtain the macro-structural constitutive response at each integration point through a nested finite element analysis, whereby the meso-structural behavior is characterized by representative volume elements (RVE).

The main drawback of this method is the large computational effort because the representative volume elements, which are usually very complex, need to be evaluated at every material point. An approach to reduce the computational effort is the concept of decoupled numerical homogenization. Therefore, a database representing the macroscopic material behavior is derived by solving the boundary value problem of the considered RVE for different applied boundary conditions. Subsequently, the approach of data-driven computational mechanics is utilized to receive an approximate solution for the boundary value problem on the macroscale with direct reference to stress-strain data obtained from mesoscale evaluations. In order to receive accurate results by data-driven analyses, a sufficient data set density with respect to the present problem is essential.

With respect to the definition of the concrete mesostructure, aleatoric uncertainties are introduced by natural variability especially in the material behavior. Additional epistemic uncertainties are caused by manufacturing tolerances and an insufficient amount of measurement data. A combined consideration is realized by polymorphic uncertainty models. The acquisition of data sets consisting of uncertain macroscopic stress-strain states leads to a large number of required evaluations of the considered RVEs and correspondingly high computational effort, which is addressed by incorporating surrogate models for uncertainty quantification. The large number of uncertainty propagations that must be performed for data set generation is the main challenge in creating the surrogates. Accordingly, overhead and training time caused by surrogate creation need to be as low as possible in order to avoid impracticably high computational cost. In this contribution, a polynomial chaos assisted data set acquisition approach enabling the efficient consideration of polymorphic uncertainty is presented and applied in the context of data-driven computational homogenization.

Human-induced vibrations of footbridges: modeling with polymorphic uncertainties

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The development of new materials allows to increase the span length of footbridges constructed as lightweight structures. However, slender footbridges are more sensitive to vibrations caused by human-induced vibrations. This can reduce the comfort for pedestrians significantly. In addition, eigenfrequencies of slender footbridges are often in the range of the step frequency. A resonance case has to be avoided to ensure the structural safety. The gait of a pedestrian and thus the step frequency is very difficult to quantify in a dynamic load model. It depends on many factors, e.g., body height and weight, gender, age, psychological aspects and even the economic and social status of a human have an influence. There are many parameters with a lack of knowledge to quantify these factors in a load model. Therefore, pedestrian load models are very simplified in current design guidelines. An adequate quantification of aleatoric and epistemic uncertainties is not yet sufficiently addressed in the modeling of human-induced vibrations of footbridges.

In this contribution, uncertain parameters for a pedestrian load model are quantified with polymorphic uncertainty models based on available data. Then, dynamic structural analyses are performed with human-induced vibrations, which are approximated by surrogate models. The results are fuzzy stochastic processes of the structural accelerations, velocities and displacements. In current design codes, the comfort levels are defined with respect to acceptable accelerations. Due to the subjective perception of structural accelerations, the comfort levels are also defined with uncertainty models. Associated results are presented for a real-world footbridge using a 3D finite element model.

Sensitivity analysis in the presence of polymorphic uncertainties based on tensor surrogates

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IGPM - RWTH

We will explore sensitivity analysis for mechanical engineering problems in presence of polymorphic uncertainty. Polymorphic uncertainty quantification allows for the incorporation of different sources of uncertainty, such as epistemic and aleatory, which have varying levels of complexity and dependence.

A measurement of distances between the most common polymorphic uncertainties will be at the core of the computation of sensitivity indices.

We will discuss how sensitivity analysis can aid in understanding the effects of input uncertainties on system performance and inform further polymorphic uncertainty quantification analysis. Additionally, we will cover methods for efficiently computing sensitivity measures for high-dimensional systems based on tensor surrogates.

A computational sensitivity analysis tool for investigations of structural analysis models of real-world engineering problems

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The method of influence functions is a well-known engineering tool in structural analysis to investigate the consequences of load variations on deflections and stress resultants. Based on its strong relationship with adjoint sensitivity analysis [1], the traditional method of influence functions can be generalized as an engineering tool for sensitivity analysis [2]. The aim of our contribution is to give insights into these methodical extensions and to demonstrate their added value.

The traditional influence function approach can be seen as work balance based on Betti's theorem. In our contribution we show how that work expression can be extended for sensitivity analysis with respect to various parameters. We discuss the significance of the resulting mechanically interpretable sensitivity analysis and its limitations. In that regard, we also specify how the graphical analysis procedure, for which the traditional influence function technique is well-known, can be generalized. The intention is to use those "sensitivity maps" to identify the positions of extreme influences and the individual effects of the partitions to the final sensitivity and its spatial distribution. In this way, structural analysis models of real-world engineering problems can be systematically explored and important model parameters to be considered in uncertainty quantification can be identified. Hence, our method has the potential to provide valuable support for preliminary investigations of structural models as a basis of polymorphic uncertainty analysis.

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The consideration of aleatory and epistemic uncertainties in the data assimilation by using a multilayered uncertainty space

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This study has been performed within the research project MuScaBlaDes "Multi scale failure analysis with polymorphic uncertainties for optimal design of rotor blades", which is part of the DFG Priority Programme (SPP 1886) "Polymorphic Uncertainty Modelling for the Numerical Design of Structures" started in 2016.

The modeling of real engineering structures is a tough challenge and always accompanied by uncertainties. Geometry, material and all boundary conditions should be quantified as accurately as possible. The quality of the numerical prediction of the system behavior and of desired system outcomes depends on the underlying model. Real measurements on the structure provide the possibility to assess and to verify the numerics. In general, discrepancies exist between the predicted and the measured values. Within the data assimilation framework, it is possible to consider both for the estimation of the system state. Additionally, the estimation of unknown parameters at once can be achieved in nonlinear problems by using the ensemble Kalman filter (EnKF).

In this contribution, the EnKF is extended by parameters, which influence the system state and which are subject to aleatory or epistemic uncertainty. These parameters have to be quantified by suitable uncertainty models first, and then integrated into the numerical simulation. Stochastic, interval and fuzzy variables are used leading to a multilayered uncertainty space and a nested numerical simulation in which the EnKF is embedded. Besides an academic example, the practical applicability is demonstrated on real engineering structures with synthetic and also with real measurement data.

Flexibility and uncertainty quantification using the solution space method for crashworthiness

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In the present landscape, researchers quantify the natural variability or lack of knowledge of a system to counteract its effects. What if, instead of trying to reduce this uncertainty, we try to exploit it during the development? In this work we propose how to use the knowledge on the said uncertainty to increase the design flexibility of the sub-systems of a new product. Imagine the development process being supported by the solution space method and its corridors on the performance of each sub-system. From a certain point of view, these corridors quantify an interval epistemic uncertainty of the development process. The method, however, allows to change the intervals while maintaining the same overall target performance. We exploit the flexibility of the method to find on which parts of the new product is worth investing to reduce the variability and which ones to allow a larger interval. A larger interval yields a bigger flexibility in the design, hence less development effort. The method we propose balances in the development process between reducing the variability of certain sub-systems and increasing the flexibility on the design of other sub-systems.

Two propagation concepts for polymorphic uncertain processes – simulation- and uncertainty quantification-based

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The combination of both types of uncertainty – aleatoric and epistemic – in polymorphic uncertainty models is common as fundamental step for a realistic description of system parameters (geometric definitions, loads, boundary conditions and material properties) in structural safety assessment. Such polymorphic uncertainty models are defined by combination of basic uncertainty models, such as random variates, interval sets, fuzzy sets etc., where the two types of uncertainty are accounted for in different basic models. As combined models, p-boxes, fuzzy probability based random variates etc. are documented.

In addition to the consideration of the two types of uncertainty, functional dependencies of uncertain quantities are observed in real world problems. Functional dependencies are due to temporal variation, referred to as uncertain process, or due to spatial variation, referred to as uncertain field.

This contribution focuses on temporally dependent polymorphic uncertainty in safety assessment of – in this application case, structural – systems. Therefore, uncertainty quantification is required, which means estimating the uncertain system responses (uncertain output) of a structural analysis (basic solution), based on the uncertain structural parameters (uncertain input). When considering polymorphic uncertain processes, a key challenge arises from the coupling and propagation of the temporal dependency in the uncertain input and in the basic solution. For this propagation, two concepts are presented.

The first concept is propagation of temporal dependency by the uncertainty analysis. Therefore, each single basic solution is not necessarily time dependent. Contrarily, the time dependency is reached by sampling from a time dependent uncertain input parameter in the uncertain analysis and each sample is applied for a single computation of the basic solution. Finally, the chaining of such basic solutions and the interdependence between them leads to time-dependent output of the total uncertainty quantification.

The second concept is propagation of time dependency in the basic solution. Therefore, each sample of the uncertainty analysis is a full realization of a time dependent function, in particular a full deterministic process. The basic solution in this concept is required to be time-dependent and the realization of the process is the deterministic input defining the function of the parameter in time.

In this contribution, both concepts are presented, and the challenges and advantages in their implementations are outlined. Moreover, general problems of polymorphic uncertainty models are pointed out based on the shown concepts and solutions for their unbiased modeling and re-sampling are introduced. As numerical examples, application cases in the simulation of the life-cycle (production process and structural operation) of compressed wood components are shown, where both concepts are applied in multiple simulation phases.

Process steering of additive manufacturing processes under polymorphic uncertainty

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During the last decade, additive manufacturing techniques have gained extensive attention. Especially extrusion-based techniques utilizing plastic, metal or even cement-based materials are widely used. Numerical simulation of additive manufacturing processes can be used to gain a more fundamental understanding of the relations between the process and material parameters on one hand and the properties of the printed product on the other hand.

Hence, the dependencies of the final structural properties on different influencing factors can be identified. Additionally, the uncertain nature of process and material parameters can be taken into account to reliably control and finally optimize the printing process. Therefore, numerical models of printing processes demand geometric flexibility while being computationally efficient.

An efficient numerical simulation of an extrusion-based printing process of concrete, applying a voxel-based finite element method is used in this study. Along with the progressing printing process, a previously generated FE mesh is activated step-by-step using a pseudo-density approach. Additionally, all material parameters vary spatially and temporally due to the time dependency of the curing process. In order to estimate material and process parameters realistically a polymorphic uncertainty approach is chosen incorporating interval-probability based random processes and fields.

By having a numerical model – at least at some level of abstraction – and an extensive description and possibility to consider uncertainties, the probabilities of the occurrence of the failure mechanisms (strength-based stability, geometric deviations, layer interface, and buckling) can be estimated. In an optimal steering of the process, failures should be minimized. However, reducing the failure probabilities of one mechanism may increase the ones of the other mechanisms, e.g., shape stability and layer interface might be in conflict.

In this study, process steering is rationalized using a reliability-based optimization approach taking into account the uncertain nature of the system's material and process parameters. In the light of polymorphic uncertainty, tailored surrogate model strategies are investigated to boost efficiency for this numerically demanding task.

MS 19 Integrating computational and experimental mechanics

Prediction and compensation of shape deviations in internal traverse grinding

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Internal traverse grinding (ITG) with electroplated cBN tools and under high speed conditions if a highly efficient process for the machining of hardened steel components. In ITG, the grinding wheel consists of a conical roughing zone and a cylindrical finishing zone. The tool is fed in axial direction into a revolving workpiece, performing roughing and finishing in a single axial stroke. Due to the process kinematics, the process forces during ITG are dependent on the current material removal rate, which varies during the process. The mechanical compliance of the entire system, consisting of both tool- and workpiece spindle, the workpiece clamping device, and all other components in the flow of force, result in shape deviations of the workpieces after machining.

We recently proposed a multi-scale simulation framework to model ITG with electroplated CBN wheels numerically [1]. A digital grinding wheel, based on real grain geometries obtained from optical measurements, was implemented in a geometric physically-based simulation (GPS) to simulate the engagement of each individual grain during the process. The normal force contributions of each individual grain were modelled by a single-grain force model, which was calibrated against two-dimensional Finite Element Simulations of single grain cuts. By taking into account both the system compliance and the total normal force, the deflection between tool and workpiece was modelled in the GPS.

Based on the simulation results, different compensation strategies for the NC tool path were implemented and compared, and a significant reduction of the shape deviations was achieved.

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Full-field validation of finite cell method computations on wire arc additive manufactured components

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Metal additive manufacturing technologies, such as wire arc additive manufacturing (WAAM), allow the manufacturing of components with maximum freedom in the geometric design and specifically adjusted functional properties. However, WAAM-produced components possess a very wavy surface that exacerbates the numerical simulation of such components. As a result, common finite element approaches with low order shape functions are not suitable for these simulations.

Instead, the finite cell method is chosen for the simulation of tube-like WAAM-produced specimens under a combined tension-torsion load. First, the contour of the specimens is determined with a portable 3D scanning technique. Then, the mechanical response of the specimens is computed using the finite cell method, where a beforehand calibrated J2-plasticity model is applied. The polynomial order of the integrated polynomials is increased for convergence studies and the mechanical response of the specimens is compared to the experimental results. During the experiments, digital image correlation measurements are performed to compare even the full-field deformation to the simulation results. Here, we choose so-called radial basis functions as a global interpolation technique to obtain the in-plane strains and stretches in the curved surfaces for both experiment as well as simulation. Since the material parameters are determined from experimental tensile testing data, uncertainties in these parameters propagate to the numerical simulations of the tube-like specimens under tension-torsion load. To consider these uncertainties when comparing the experimental with the numerical results, the Gaussian error propagation is applied for estimating the uncertainty in the mechanical response.

On the influence of microscale defects on electrical properties: nanoscale experiments and multiscale simulations

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Computational multiscale methods are well-established tools to predict and analyse material behaviour across scales. They are applied so as to reveal the influence of the underlying microstructure on effective material properties and enable complex multi-physics interactions to be accounted for in simulations. Whereas multiscale approaches for thermo-mechanical problems and electro-active solids have been in the focus of intense research in the past decade, rather few works have so far focused on electrical conductors.

Based on the recent works [1,2] this material class and, in particular, the influence of mechanically-induced microscale defects on the effective conductivity is subject of the present contribution. At the outset of the developments, a quasi-stationary setting is assumed such that Maxwell's equations reduce to the continuity equation for the electric charge and to Faraday's law of induction. Scale-bridging relations for the kinematic- and flux-type quantities are established, their consistency with an extended Hill-Mandel condition is shown and a closed-form solution for the effective macroscale conductivity tensor based on the underlying microscale boundary value problem is provided.

In view of the experimental investigations [3,4] the effective conductivity tensor, as a fingerprint of the material microstructure, is of primary interest. To study the applicability of the proposed approach, focused ion beam milling is used in a first step to generate geometrically well-defined microstructures [4]. In a second step, focus is laid on mechanically-induced micro-cracks in metal thin films [3]. Both sets of microstructures are electrically characterised by means of four point probe resistance measurements and analysed by means of the proposed computational multiscale scheme. Good accordance between experiment and simulation is achieved which shows the applicability of the proposed multiscale formulation.

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Experimental and simulative fatigue strength studies of laser beam welded copper connections based on the real geometry

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The recording and evaluation of component life in electric drive systems is considerably complicated by the newly used materials and material compositions. Particularly critical are electrical subcomponents which have beam welded connections made of high-purity copper. Due to the strong coupling between stress and strength as well as the novel material properties, established methods of weld strength analysis cannot be applied without restriction. Therefore, an adapted procedure for the evaluation of the fatigue properties of these junctions is to be developed with the aim of a computational proof of service life under high-frequency vibration loads in the VHCF range.

The aim of the talk is to present the complex and thermally determined properties of the special welding spot and the inherent fatigue properties. On the one hand, the extensive and variable test program in relation to the investigated impact types as well as initial sheet configurations will be discussed. On the other hand, a self-contained methodology is to be presented, which guarantees the transferability of the simulatively determined strength between different welded joints. It is based on the NuMeSis method presented by KAFFENBERGER [1], which evaluates the specific, static notch stress situation based on real measured weld seam geometries of steel components. The transferability of the fatigue strength between different welded joints is then achieved by the combined consideration of the micro-support effect according to NEUBER [2] and the weakest link model according to WEIBULL [3]. The transfer of this method from statically loaded steel welds to high-frequency loaded copper welds requires both the embedding of the method in the methodologies of computational vibration fatigue as well as profound numerical changes of the method. This guarantees an efficient, automated evaluation and the consideration of the special properties of the high-purity copper material. Together with other influencing factors such as the presence of internal defects, this procedure leads to a self-contained evaluation concept for welded copper compounds.

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A closer look at isotropic hardening - modeling and experiments

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Although isotropic hardening plasticity is the most basic hardening type in material modeling, many existing models rely on an overly simplistic hypothesis: a direct relationship between yield stress and accumulated plasticity. Our recent publication [1] falsifies this hypothesis for one medium carbon steel. Furthermore, we investigated the yield surface evolution and its relation to the accumulated plasticity. Several distortional hardening models in the literature assume a direct relationship between the complete yield surface evolution and accumulated plasticity for uniaxial cyclic loading.

These identified modeling deficiencies underscore the necessity for new constitutive models. To tackle this need, we propose a novel plasticity formulation incorporating neural networks in a thermodynamically consistent framework. We extract and analyze the trained neural networks to identify new constitutive equations with sparse regression techniques, cf. [2]. The complete process results in the discovery of new evolution equations based on the experimental data. A notable finding is new interactions between the hidden state variables in the evolution laws. Based on these equations, we can design new specialized experiments to further understand the interplay between loading type and hardening behavior.

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Modeling glass above the glass transition temperature by means of a thermo-mechanically coupled material model for large deformations

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The field of application of thin glass products is vast including various engineering branches such as e.g. electronics, medical equipment and automobiles. In order to realize a cost-efficient production of surface shapes with high accuracy and complexity, a novel replicative glass processing technique called non-isothermal glass molding has been developed (see [1]). However, the production of thin glass components using this technology still raises the issue of shape distortions, cracks and surface defects of molded parts. Therefore, the experimental investigation and mechanical modeling of glass above the glass transition temperature at finite strains are combined in order to simulate these glass forming processes.

Previous experimental studies have shown that the material behavior can be predicted adequately by the Maxwell model (see e.g. [2]). Based on this viscoelastic formulation (see [3]), the material law used is thermo-mechanically consistent and allows the prediction of rheological effects observed during the experiments. In particular, a stress-dependent relaxation time is used to describe the relaxation behavior and the dissipation generated is also taken into account. Regarding the experimental investigation, isothermal uniaxial compression tests above the glass transition temperature are performed for different strain rates and temperatures. By combining the experimental data with the simulation, a multi-curve-fitting is introduced. This nonlinear optimization lead to suitable material parameters with respect to distinct temperatures.

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An anisotropic crack initiation criterion for highly deformed R260 rail steel: experiments and numerical simulations

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Accumulation of plastic deformation in the surface layer of rails and wheels during many rolling contact loading cycles can result in fatigue crack initiation. The behavior and strength of this highly deformed and anisotropic layer are thus key properties of a rail or wheel material. Establishing crack initiation criteria that account for the properties of the material and are experimentally validated is of great importance in railway engineering.

In this contribution, test results from previously conducted axial-torsion experiments on pearlitic R260 steel specimens have been used to assess the accuracy of available crack initiation criteria as well as to suggest modified criteria. In the experiments, solid test bars were predeformed by torsion under different nominal axial stresses to replicate the anisotropic material in the surface layer of rails. Some of the predeformed specimens were re-machined into a thin-walled tubular shape and then subjected to further cyclic multiaxial loading.

Various crack initiation criteria for rolling-contact situations have been proposed in the literature. However, anisotropy has not been considered in many of them, or they are limited to a specific loading condition, or they are not based on experimental data. In this contribution, we predict the cyclic plasticity and anisotropy evolution during the tests by using a finite strain plasticity model and FEM. Then, by using the obtained stress and strain histories, several crack initiation criteria are evaluated as a post-processing step and further improved by considering the effect of anisotropy.

An experimental validation of topology optimization for materials with hardening

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It is still challenging in the field of topology optimization to optimize structures including the complex real-world material behavior. Nevertheless, the specific material behavior has significant influence on the optimal results. Therefore, we proposed a numerical efficient surrogate model for plasticity including hardening extending the established thermodynamic topology optimization (TTO). Even if the simulation results seem reasonable, experimental validation is still mandatory to ensure feasibility for real-world application.

Thus, we present the validation of the thermodynamic topology optimization including plasticity with hardening by comparison of experiments with optimization results. To this end, topology optimized structures are manufactured by additive manufacturing. The real material behavior needs to be determined from additively manufactured tensile specimens so that the material parameters for the specific hardening are considered during the optimization process. Subsequently, structures with respect to hardening as well as elastically reference are optimized and manufactured. Optimization results with pure elastic and plastic model are compared by experiments to show the importance of including hardening behavior within optimization for real-world application.

A nonlocal model for damage-induced anisotropy in concrete

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A better understanding of the stress-deformation behavior of concrete structures under different loading and environmental conditions is inevitable to maintain the structural integrity and to avoid catastrophic failures. In the framework of continuum damage mechanics, several material models have been developed in the past to investigate the constitutive response of concrete under different conditions. It has been observed from the experimental studies that the elastic response and stiffness degradation of concrete are dependent on the orientation of micro-cracks and direction of applied loading. This necessitates the incorporation of damage-induced anisotropy[1] in material models for concrete.

In this regard, an anisotropic damage model that describes the softening response of concrete under different loading conditions is developed applying finite element formulations. A two dimensional damage effect tensor is employed to describe the anisotropic evolution of damage. Damage models that take account of the softening responses are known for their spurious mesh dependencies. An implicit gradient enhancement technique introducing an internal length scale is implemented to overcome the numerical difficulties due to damage localization[2]. The model is verified, calibrated and validated considering various experimental results from the literature including monotonic and cyclic loading cases with different load patterns.

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Bayesian finite element model updating using full-field measurements of displacements

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Finite element (FE) models are widely used to capture the mechanical behavior of structures. Uncertainties in the underlying physics and unknown parameters of such models can heavily impact their performance. Thus, to satisfy high precision and reliability requirements, the performance of such models is often validated using experimental data. In such model updating processes, uncertainties in the incoming measurements should be accounted for, as well. In this context, Bayesian methods have been recognized as a powerful tool for addressing different types of uncertainties.

Quasi-brittle materials subjected to damage pose a further challenge due to the increased uncertainty and complexity involved in modeling crack propagation effects. In this respect, techniques such as Digital Image Correlation (DIC) can provide full-field displacement measurements that are able to reflect the crack path up to a certain accuracy. In this study, DIC-based full field measurements are incorporated into a finite element model updating approach, to calibrate unknown/uncertain parameters of an ansatz constitutive model. In contrast to the standard FEMU, where measured displacements are compared to the displacements from the FE model response, in the force-version of the standard FEMU, termed FEMU-F, displacements are applied as Dirichlet constraints. This enables the evaluation of the internal forces, which are then compared to measured external forces, thus quantifying the fulfillment of the momentum balance equation as a metric for the model discrepancy. In the present work, the FEMU-F approach is further equipped with a Bayesian technique that accounts for uncertainties in the measured displacements, as well. Via this modification, displacements are treated as unknown variables to be subsequently identified, while they are allowed to deviate from the measured values up to a certain measurement accuracy. To be able to identify many unknown variables; including constitutive parameters and the aforementioned displacements, an approximative variational Bayesian technique is utilized.

A numerical example of a three-point bending case study is presented first to demonstrate the effectiveness of the proposed approach. The parameters of a gradient-enhanced damage material model are identified using noisy synthetic data, and the effect of measurement noise is studied. The ability of the suggested approach on identifying constitutive parameters is then validated using real experimental data from a three-point bending test. The full field displacements required as input to the inference setup are extracted through a digital image correlation (DIC) analysis of the provided raw images.

MS 20 Reduced order modeling and fast simulation strategies

Combination of data-based model reduction and reanalysis to accelerate structural analysis

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In many applications in Computer Aided Engineering, like parametric studies, structural optimization or virtual material design, a large number of almost similar models have to be simulated. Although the individual scenarios may differ only slightly in both space and time, the same effort is invested for every single new simulation with no account for experience and knowledge from previous simulations. Therefore, we have developed a method that combines data-based Model Order Reduction (MOR) and reanalysis, thus exploiting knowledge from previous simulation runs to accelerate computations in multi-query contexts. While MOR allows reducing model fidelity in space and time without significantly deteriorating accuracy, reanalysis uses results from previous computations as a predictor or preconditioner.

The workflow of our method, named Reduced Model Reanalysis (RMR), is divided into an offline and online phase. In the offline phase, data are generated to cover a wide range of the parameter space. From this data a surrogate model is learned in a reduced space using regression algorithms from the field of machine learning. Depending on the requirements of the system, different regression algorithms are favorable, e.g. linear regression, a k-nearest neighbor algorithm, a neural network, or a Gaussian process. The models are learned in the reduced space due to the prohibitively large number of degrees of freedom of the full finite element model. The reduced subspaces are obtained via a snapshot POD (proper orthogonal decomposition). In the online phase, approximations of all relevant solution quantities are obtained from the surrogate model. Their projection to the full space provides predictors that allow for an accelerated solution of the system in comparison to a standard structural mechanics computation.

In the case of nonlinear stability analysis this method can for example be used to accelerate the exact computation of critical points by the method of extended systems. Data generation in the offline phase is also accelerated by a newly developed adaptive time stepping scheme. With this scheme the number of steps to approach critical points with a path following scheme can be significantly reduced. Further potential fields of application of RMR are general nonlinear static and transient problems, with particular challenges as soon as path-dependence comes into play.

Scientific machine learning for affordable high-fidelity simulations of metal additive manufacturing

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Metal additive manufacturing (MAM) has received significant attention in recent years due to its significant advantages such as increased design flexibility for complex geometries, shorter production-cycle, and efficient use of raw materials. To fully realize the potential of MAM in the context of Industry 4.0, it is necessary to address challenges related to the mechanical reliability of printed parts and their associated costs. Currently, trial-and-error methods are the most common way of optimizing MAM process conditions for achieving the desired printing quality. Meanwhile, numerical simulations can provide a more profound understanding of the physical phenomena involved in the build process, leading to a more systematic optimization of process conditions, and ultimately making the 'first-time-right' high-quality production possible. Achieving a thorough quantitative understanding of the process requires insights from models covering various physical aspects including thermal, mechanical, metallurgical, and fluid-dynamics interactions. However, high-fidelity simulations of such models are accompanied by significant computational costs and therefore have limits in applications, particularly in sensitivity and optimization analyses where solutions for a wide range of scenarios are required.

To address this challenge, we initiated a project in 2021, with the support of the Swiss National Science Foundation (SNSF), to explore the feasibility of meaningful acceleration of these simulations without significant compromise in accuracy and reliability. Specifically, the project aims to develop solutions for thermal, microstructure, and residual stress simulations for the laser powder bed fusion (LPBF) process. To generate experimental validation data, Hastelloy X serve as the 'model material'. An overview of the results obtained so far, focusing on thermal and microstructure simulations, are presented.

Several techniques have been examined to reduce the computational cost of thermal simulation for LPBF, including a multi-scale simulation strategy, surrogate modelling, and physics-informed neural networks (PINNs), where the advantages and limitations of each approach are discussed. In the field of microstructure modelling, a 'Neural Cellular Automata' method has been developed, which outperforms the conventional Cellular Automata with up to 6 orders of magnitude acceleration in computation speed. Moving forward, the project will continue with a focus on the development of affordable high-fidelity models of residual stress development until 2025.

An efficient integration split of geometric and material nonlinearities

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Modeling for the description and prediction of processes in nature often leads to partial differential equations. Solving these field equations can only be done analytically in very few cases, so that in practice numerical approximation methods are often used. Variational methods like the Galerkin method have proven to be very effective and are widely used in industry and research. To set up the system of equations, integration over the area to be calculated is necessary. For more complex geometries or nonlinear equations, analytical integration becomes difficult or even infeasible, so that integration is also often performed numerically in the form of weighted evaluations of the integrand, the Gauss quadrature. In order to benefit from the quasi-optimal accuracy of the Galerkin method according to Cea's lemma in the linear case, the quadrature scheme must also be of sufficient accuracy. On the contrary, for more complex constitutive laws, under-integration is often used in engineering to save computational time. Based on a split of geometric and material nonlinearities, the present talk introduces a one-point integration scheme that is able to integrate polynomial shape functions of arbitrary order geometrically accurate. The material nonlinearity can be captured with the desired accuracy via a Taylor series expansion from the nonlinear state. As a demonstration the integration scheme is applied to two-dimensional polygonal shaped second order virtual elements where the quadratic projection is integrated via a single integration point.

A nonlinear reduced order modelling approach to solid mechanics with application to representative volume elements

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Manifold learning techniques such as Laplacian Eigenmaps (LE) [1] are commonly applied in fields like image and speech processing, to extract nonlinear trends from large sets of high-dimensional data [2]. Such techniques are also intriguing as model order reduction methods in multiscale solid mechanics: LE can capture nonlinearities in the solution manifolds of discretised physical problems [3]. Compared to POD-based algorithms, this may result in reduced order models yielding more accurate results with fewer parameters and lower computational effort [3]. Consequently, manifold learning techniques have been applied successfully to problems in fluid mechanics [3] and elastodynamics [4].

In the framework of the FE^2 method – in which computations on microscale representative volume elements (RVEs) are performed at each Gauss point of a macroscopic problem [5] – the payoff of such computational cost reduction may also be significant.

This contribution discusses the application of LE to model order reduction for RVE computations. Nonlinear, hyperelastic and elastoplastic behaviour is considered. The area of application comes with unique challenges and opportunities: for example, the mapping between reduced and original spaces and the projection of residuals onto reduced bases is not trivial [3]. On the other hand, the underlying PDEs [4] and the parametrisation of the RVE problem via a macroscopic deformation gradient and history variables [5] imply a strong (nonlinear) correlation in the unknown displacement degrees of freedom to be reduced. This talk will explore some of these challenges and opportunities.

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Reduced order modeling for second-order computational homogenization

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Multiscale methods are often employed to study the effect of microstructure on macroscopic behaviour. For non-linear problems, these usually result in a two-scale formulation, where macro- and microstructure are simultaneously solved and coupled. If the microstructural features are much smaller compared to the macrostructural size, its effective behavior can be sufficiently predicted with first-order computational homogenization. However, if scale separation cannot be assumed or non-local effects due to buckling, softening, etc., emerge, higher-order methods, such as second-order homogenization [1], need to be considered. This formulation contains the second gradient of the displacement field, giving rise to a length-scale associated with the length-scale of the underlying unit cell, thus making it possible to capture size and non-local effects. Solving such problems is currently computationally expensive and typically infeasible for realistic applications, which limits the applicability of this method.

In this work, we address this issue by developing a reduced order model for second-order computational homogenization scheme based on Proper Orthogonal Decomposition. We consider different numerical examples and discuss different training strategies, computational savings and accuracy of the surrogate model.

Acknowledgements: This result is part of a project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 Research and Innovation Programme (Grant Agreement No. 818473).

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Benchmarking the performance of Deep Material Network implementations

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The availability of high quality µ-CT images of materials allows for detailed multiscale simulation workflows in digital material characterization. In this case, data driven hybrid machine learning approaches are used to speed up full field approaches. Efficient and performance implementations of such data driven methods are essential for them being used for industrial applications.

This work concerns DMN (Deep Material Network) whose potential applications were exploited recently [1,2,3]. They only need linear elastic training data to identify equivalent laminate microstructure, which can be used to predict nonlinear behavior.

The industrial applicability of the DMN for short fiber reinforced plastic is investigated by comparing its speed and accuracy against direct numerical simulation results[4,5] on RVEs[6] using different physically nonlinear material behavior.

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Reduced order modeling of shallow water equations using a machine learning based non-intrusive method

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Reduced Order Models (ROMs) have been widely used to efficiently solve large-scale problems in many fields including computational fluid dynamics (CFD) [1]. ROMs techniques allow to replace the expansive Full Order Model (FOM), by a ROM that captures the essential features of the system while significantly reducing the computational cost. In this work, we draw inspiration from [2] to implement a reduced basis (RB) method for model reduction of the Shallow Water Equations (SWEs) using Proper Orthogonal Decomposition (POD) and Artificial Neural Networks (ANNs). This method, referred to as POD-NN, starts with the POD technique to construct a reduced basis, and then makes us of an ANN to learn the associated coefficients in the reduced basis. It follows an offline-online strategy: the POD reduced basis along with the training of the ANN are performed in an offline stage, and then the surrogate model can be used for hyper-fast predictions. The process is non-intrusive since it does not require opening the black box of the FOM. The developed method is tested [3] on a real data set aiming at simulating an inundation of the Aude river (Southern France). The results show that the proposed method can achieve significant computational savings while maintaining satisfactory accuracy on the hydraulic variables of interest compared to the full-order hydraulic model. The proposed method is able to capture the key features of the SWEs in particular the wave propagation. Overall, the proposed non-intrusive POD-NN method offers a promising approach for ROM of SWEs while being affordable in view of fast real time inundation simulations.

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Fast approximation of fiber reinforced injection molding

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Discontinuous fiber reinforced composites are used in many application areas ranging from automotive to healthcare. Such parts are often manufactured in and injection molding process, as it is an economical process for high volume markets. The simulation of the injection molding process is well established and specific commercial tools have been developed for this task. However, the transient solution of the underlying non-linear multi-phase flow is computationally expensive and computation may take multiple hours for complex geometries. This computational time is prohibitively large for computational optimization of the product design or the process parameters. Hence, we propose a two-step process to accelerate the mold filling prediction: i) Solve a modified Eikonal equation to compute distance maps to the injection gate and nearest walls. This is computationally cheap, as it is only a stationary equation to solve. ii) Train feed forward neural networks to obtain a data-driven relation between the encoded distance maps and mold filling features, such as fill time and fiber orientation. We sample a set of geometries, automatically generate CAD models, and simulate these in a commercial injection molding solver to build a training data set. Subsequently, we apply different feed forward neural network architectures and evaluate their performance.

Geometry-based approximation of waves in complex domains

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Let us consider wave propagation problems over 2-dimensional domains with piecewise-linear boundaries, possibly including scatterers. Under some assumptions on the initial conditions and forcing terms, we have proposed an approximation of the propagating wave as the sum of some special nonlinear space-time functions. Each term in this sum identifies a particular ray, modeling the result of a single reflection or diffraction effect. In this talk I will describe an algorithm for identifying such rays automatically, based on the domain geometry.

To showcase our proposed method, I will present several numerical examples, such as waves scattering off wedges and waves propagating through a room in presence of obstacles.

Efficient isogeometric analysis of lattice structures

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Additive Manufacturing (AM) and especially its metal variants constitute today a reality for the fabrication of high-performance industrial components. In particular, AM allows the construction of novel cellular structures, the so-called lattices, where well-designed unit cells are periodically repeated over a macro-shape to achieve exceptional specific performances, such as unprecedent stiffness-to-weight ratios. These structures, however, are very difficult to simulate numerically: on the one hand, the application of multiscale methods based on homogenization appears delicate due to an insufficient separation of scales (macro versus cell scales); on the other hand, solving directly the high-fidelity, fine-scale problem requires handling large numbers of complex cells which is often intractable if standard methods are blindly used. As a solution, immersed domain techniques have been applied, but such methods, generic in terms of applications, may not be optimal in the case of lattices.

In this context, the purpose of this work is to develop a HPC algorithm dedicated to lattices that takes advantage of the geometric proximity of the different cells in the numerical solution. In order to do so, we start by adopting the CAD paradigm based on spline composition along with its corresponding IGA framework. This offers (i) great flexibility to design any lattice geometry and (ii) fast multiscale assembly of the IGA system. Then, we resort to the family of Domain Decomposition solvers, and develop an inexact FETI based algorithm that avoids solving numerous local cell-wise systems. More precisely, we extract the “principal” local cell stiffnesses using a greedy approach, and use the latter as a reduced basis to efficiently solve all the cell-wise systems. It results in a scalable algorithm that tends to be matrix-free. During the talk, a range of numerical examples in 2D and 3D will be presented to account for the efficiency of our method both in terms of memory and computational cost reduction.

Analyzing discrete dislocation dynamics using data-driven approaches

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Plasticity is the result of the motion and interaction of discrete dislocations in a crystalline material. Modelling plasticity at the crystal level based on discrete dislocation dynamics (DDD) is challenging due to the complexities associated with the dislocation activities of different slip planes. A data-driven approach provides an alternative method for simulating the complex behavior associated with plasticity at a small scale. We use methods based on dynamic mode decomposition1 (DMD) to analyze the DDD data2. We built reduced-order models for describing system dynamics with a few dominant modes. The models are built upon datasets of different physical resolution, e.g. dislocation density information resolved on the slip system level based on total dislocation densities, dislocation density vectors, or second-order dislocation alignment tensors. Different levels of spatial resolution are used to evaluate the effectiveness of models in reconstruction of the analysed data.

The modelling approach is then extended to forecast material response beyond the training dataset, for which we adopt more general (non-linear) Koopman operator theory and advanced stabilized DMD schemes, like shift invariant (physically informed) DMD or optimized DMD3. The different schemes are compared in their ability to predict the nonlinear behaviour in crystal plasticity from the DDD data.

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Localized reduced order models in isogeometric analysis

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This contribution is motivated by the combined advantages of an integrated framework from CAD geometries to simulation in real time. In a typical workflow for design and shape optimization, multiple simulations are required for all possible designs represented by different geometrical parameters. This might entail a high computational cost in particular for real world, engineering applications. The development of efficient reduced order models that enable fast parametric analysis is essential for such applications. At the same time, the capabilities of splines and isogeometric analysis allow for flexible geometric design and higher-order continuity in the analysis. In CAD design, trimmed multi-patch geometries are widely used to represent complex shapes. The presence of geometric parameters introduces challenges for efficient reduced order modeling of problems formulated on such unfitted geometries. We propose a localized reduced basis method to circumvent the shortcomings of standard reduced order models in this context [1]. In this talk we present the developed strategy and address fast parametric analysis of problems in structural mechanics. The construction of efficient reduced order models for geometries described by multiple trimmed patches as well as their use in parametric shape optimization will be discussed. Numerical examples will be presented to demonstrate the accuracy and computational efficiency of the method.

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MS 21 General

The redundancy matrix as an alternative measure for the assessment of structures

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Redundancy, and thus the degree of static indeterminacy, plays an important role in the design of structural systems. According to Linkwitz and Ströbel, the distribution of static indeterminacy in the system can be described by the redundancy matrix. The redundancy contribution of an 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 statical indeterminacy of the entire structure. The extension of Ströbel's notion for discrete truss systems to frames and continua can provide valuable insight into the load-bearing properties of a structure and has the potential to become an exciting new branch in the classical field of structural analysis.

Obviously, statical indeterminacy and its distribution in a structure have a decisive influence on the structural behavior. Therefore, the redundancy matrix can be a good measure to understand and evaluate structural behavior. It can also be used for robust design optimization and assessment of imperfection sensitivity during the assembly process.

The computation of the redundancy matrix generally requires a high effort due to the necessity of expensive matrix operations. A closed-form expression for the redundancy matrix can be derived via a factorization that is based on singular value decomposition. For moderately redundant systems it proves to be computationally very efficient. For small modifications of the structure, such as adding, removing, and swapping elements, generic algebraic formulations can be derived for efficiently updating the redundancy matrix.

While the redundancy matrix concept has only been applied to linear analysis, it can be extended to the nonlinear regime. In this case, the contribution of the nonlinear load transfer can be analyzed separately. Furthermore, the redundancy matrix allows for a simple extension of the notion of static indeterminacy to nonlinear analysis.

Hygro-thermo-mechanical influences on the service life of rate-dependent hyperelastic adhesives

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Semi-structural bonded joints of steel components are exposed to long-term stresses due to water diffusion, temperature change and external forces during operation load cases. This hygro-thermomechanical loadingprocesses lead to successive degradation of stiffness and strength due to material damage resulting from chemical aging and fatigue processes. This material deterioration causes finally complete failure of the adhesive bonding and determines the service life. In the following contribution, a methodology is presented to predict the service life of hygro-thermo-mechanically loaded semistructural adhesive joints by transient FE simulation. The lifetime prediction is based on the concept of finite-viscoelasticity and a damage. The first part of the finite-viscoelastic material theory consists a generalized Maxwell body together with a Neo-Hooke model, in which the effects of temperature and humidity changes on the viscoelastic properties of the adhesive bond are captured by the time-temperature and time-water concentration shifts. The second part for material damage is an ordinary differential equation for the void evolution. It consists of a creep and a moisture damage part for the damage developments, caused by the local water concentration due to mechanical stress and chemical aging. Both damage parts are multiplied by an Arrhenius-type functions to account for the effect of temperature and concentration on the defect growth. The local water concentration in the adhesive is calculated by Fick's model, based on a concentration boundary condition. The diffusion parameters are determined from gravimetric tests. The interaction of the creep and the moisture damage parts is studied by using analytical and numerical solutions of the damage evolution equation. All parameters of the damage model are determined by using fracture times from creep tests under different climatic conditions and loading levels. The validation of the material model, the damage approach and the identified parameters are carried out by means of experimental large component tests, which are compared with the simulation results.

Crack tip loading and crack growth analyses using the virtual element method

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To precisely model crack growth, accurate calculations of crack front loading and crack deflection angles are essential. These calculations require solutions of the underlying boundary value problems (BVPs), which are typically obtained by applying numerical methods, e.g., the finite element method (FEM). However, since accuracy and computational cost of the analyses are in general competing aspects, compromises often must be made to generate satisfactory results in acceptable times. In contrast, the use of more efficient methods, both for the solution of the BVP as well as for the subsequent crack tip loading analyses, can substantially lower the computational effort while maintaining desired accuracies. The virtual element method (VEM) is a fairly new discretization scheme for the numerical solution of BVPs, and can be interpreted as a generalization of the FEM. Since the VEM can handle arbitrary polytopal meshes in a straightforward manner, it provides a higher degree of flexibility in the discretization process than the FEM, which turns out to be profitable in terms of both computing times and accuracy.

In the context of numerical applications of fracture mechanics, the probably most attractive feature of the VEM results from the possibility to employ elements of complex shapes, which may be convex as well as concave. Consequently, crack growth simulations benefit from the fact that incremental changes in the geometry of a crack do not require any remeshing of the structure, but rather crack paths can run through already existing elements. Although the method has already proved to provide an efficient tool for crack growth simulations in plane problems, there is still further research required regarding the efficient and precise evaluation of crack front loading quantities and the extension towards spatial crack problems.

This work aims to discuss aspects of the virtual element method for crack tip loading analyses and crack growth simulations. Classical as well as advanced concepts of numerical fracture mechanics are adopted and implemented in connection with the VEM, carefully investigating and exploiting the advantages and opportunities the discretization method offers in this regard. Crack growth simulations based on the VEM are performed and results are compared to reference solutions as well as solutions obtained by the FEM.

Kirchhoff-Love shells in scaled boundary isogeometric analysis for smooth multi-patch structures

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In modern applications of computer-aided design (CAD) for the analysis of shell structures, isogeometric analysis (IGA) is a powerful tool to incorporate both design and analysis. However, when it comes to multi-patch structures, C1-continuity across patches is not naturally fulfilled and computation of Kirchhoff-Love shells is not straightforward since well-defined second-order derivatives are necessary for the analysis. Furthermore, trimming is a major problem as the mathematical underlying of the CAD surface is not inherently suitable for standard IGA.

The approach presented in this talk deals with a Kirchhoff-Love shell formulation in the framework of scaled boundary isogeometric analysis [1,2] with C1-coupling. In scaled boundary (SB), the domain is described by its boundary and scaled to a scaling center, which we denote as an SB block. Thereby, each SB block consists of several IGA patches. This has the advantage of being applicable to multi-patch structures with various numbers of edges or boundaries. Besides, a possible trimming curve is easily incorporated into the boundary representation. The domain can be subdivided into several SB blocks to obtain star convexity. However, even for a single SB block, C1-continuity is not fulfilled across the IGA patches within the SB block. To show the feasibility of the coupling approach involving SB parametrizations, it heeds the concept of analysis-suitable G1 parametrizations [3] combined with special consideration of the basis functions in the scaling center. The method is especially powerful when it comes to complex geometries that cannot be described by a single IGA patch which is outlined in several examples.

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On the implementation of a dual lumping scheme for isogeometric element formulations

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Isogeometric analysis (IGA) employs higher order polynomial shape functions, which are directly extracted from the CAD model. Unlike the standard Finite Element Method (FEM), which commonly uses Lagrange basis functions, IGA typically uses Non-Uniform Rational B-Splines (NURBS) or other types of splines. The use of spline-based FEM results in efficient computations with a relatively small number of elements, as increasing the order of NURBS basis functions enhances the convergence rate.

In the field of IGA, using high polynomial orders results in precise computations for structures that are exposed to static and dynamic loads. However, this also leads to highly accurate mass matrices with large bandwidths, resulting in increased computational effort, particularly for explicit dynamic analysis with a large number of time steps. To address computational efficiency, mass lumping techniques are commonly applied to achieve diagonal mass matrices, reducing the inversion of the mass matrix to a simple reciprocal operation. Many mass lumping schemes have been developed over time, but commonly the row-sum technique is attracted. These techniques were primarily invented fitting the requirements of standard FEM. Unfortunately, they deteriorate the convincing convergence rates of IGA when high polynomial orders are employed. Therefore, a lumping scheme tailored to IGA formulations using higher-order basis functions is necessary for efficient dynamic computations.

This study proposes the usage of dual basis functions as test functions in IGA element formulations with NURBS shape functions. By incorporating dual test functions, the Bubnov-Galerkin formulation is transferred to a Petrov-Galerkin formulation, resulting in non-symmetric stiffness matrices and - as effect of the duality - consistent diagonal mass matrices. For the presented formulation only dual basis functions are considered, which can be constructed by a combination of the initial NURBS shape functions. Hence, the changes by the dual formulation on element level can be shifted to an afterwards modification of the global matrices obtained from common IGA formulations. Thus, implementing this technique in existing codes is straightforward. Numerical examples demonstrate the efficiency of the dual approach compared to existing methods.

Isogeometric contact with plastic materials

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Simulations for predicting critical process variables in machining applications have been carried out for years. One important simulation-based analysis class in this context is the Finite Element Method (FEM). It is challenging to model the process with FEM as the metal is subjected to extensive deformation at high strain rates and temperatures. This large deformation is primarily irreversible and requires a plastic material model. The so-called orthogonal cutting process is a good abstraction of machining applications, where only a 2D representation is considered. It involves a tool cutting through a workpiece, forming chips. The shape of these chips is a crucial validation criterion for the accuracy of the simulation. One way to improve the representation of geometries in FEM simulations is to utilize Isogeometric Analysis (IGA), where the classical Lagrangian basis functions are replaced by the basis of Non-Uniform Rational B-Splines (NURBS). As these splines are commonly used for the representation of geometries in CAD models, IGA bridges the analysis with the initial design geometry.

The workpiece is modeled with a plastic material model, the Johnson-Cook hardening model, which includes a strain-rate dependency. Another crucial detail to model is the contact between the tool and the workpiece. In this work, we model the tool as a rigid B-Spline and employ a penalty contact formulation. Our focus is to investigate the influence of employing Isogeometric Analysis for the chip-forming process and the resulting chips. Furthermore, we compare the results to a classical FEM approach.

Computational study of mesh-influences in the explicit Material Point Method

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The finite element method can become susceptible to mesh distortion and numerical instabilities at huge deformations. As an alternative numerical method, the Material Point Method (MPM) can be used for this purpose, combining the advantages of the Lagrangian description of the bodies while solving the equations of interest on the Eulerian grid, see [1]. In the MPM, bodies are discretized as material points while their mechanical properties are mapped to the background grid on which the equations are solved. In this contribution, numerical examples are presented that are subject to large deformations in the context of dynamic processes. These examples exhibit a kind of mesh-dependence in different quantities. Therefore, the focus of this contribution is on the improvement and increase in stability of the numerical results, which is achieved by translations of the grid. Within this method, the origin of the background grid is shifted randomly at the beginning of each time step in a small manner in each direction. This shifting procedure can be interpreted as smearing the grid over time, eliminating the mesh-dependence shown in the resulting quantities.

References:

[1] D. Sulsky, Z. Chen und H. Schreyer. “A particle method for history-dependent materials”. In: Comput. Method Appl. M. 118.1-2 (1994), S. 179-196. doi: 10.1016/0045-7825(94)90112-0.

Mixed convection flow over a heated or cooled horizontal plate

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The present study concerns the laminar mixed convection flow over a heated or cooled horizontal plate of finite length at a zero angle of attack and a small Richardson number. The plate is located either in a channel or in a semi-infinite space behind a flow straightener. In the limit of a small Prandtl number, these conditions correspond to the boundary-layer solutions of Müllner and Schneider (2010), and Schneider (2000), respectively.

The hydrostatic pressure difference between the plate's lower and upper sides and the Kutta condition at the trailing edge induce a circulation with a global effect on the flow around the plate. In contrast to the classical aerodynamics problem of an isothermal flow around an inclined plate, the thermal wake also contributes to the circulation in the outer flow. This circulation can lead to flow separation at the bottom side of a heated plate (or an upper side of a cooled plate) when the Richardson number exceeds a certain threshold, depending on the Reynolds and Prandtl numbers.

The steady two-dimensional solution of the governing equations under the Boussinesq approximation is computed with the Finite Element solver FEniCS. Goal-oriented adaptive mesh refinement is employed in order to resolve both the viscous and the thermal boundary layers.

In the talk, the numerical solution will be compared to the boundary-layer solutions. The effect of the governing parameters on the flow will be investigated, also beyond the range of validity of the boundary-layer solutions. For a plate inside a channel, the flow separates close to the leading edge even for relatively low values of the Richardson number. The threshold Richardson number for separation decreases with increasing Reynolds number. For certain parameters, multiple steady two-dimensional solutions come into existence, differing by the size of the separation bubble. We show that the separation can be suppressed by bending a short leading section of the plate. Finally, we consider the effect of a heat source at the leading edge of a cooled plate.

References

M. Müllner and W. Schneider, Heat Mass Transf. 46, 1097-1110 (2010)

W. Schneider, Proc. 3rd Eur. Therm. Sci. Conf., 195-198 (2000)

A virtual element method for three-dimensional contact with non-conforming interface meshes

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MS

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The virtual element method (VEM) has been demonstrated to be effective in a variety of engineering problems. In recent years, it has gained high interest in both mathematics and engineering communities. In this work, a low order virtual element method for the treatment of three-dimensional contact problems with non-conforming interface meshes is presented. The contact conditions can be employed on different enforcing strategies. For non-conforming meshes, a node-to-surface enforcement leads to wrong force distributions at the contact interface. Here, we utilise a mesh adaptivity strategy, which leads to conforming meshes at the contact interface, without introducing new elements or changing the ansatz. In fact, we take advantage of the useful feature of the virtual element method, which allows to introduce new topological nodes during the simulation. It allows to employ a very simple node-to-node contact formulation for the treatment of contact. Thus, this work presents a simple geometrical approach to cut element faces and introduce new nodes into the existing mesh. Beside a node-to-node contact formulation, this also allows to treat the contact pairs as polygonal pairs and thus to use a surface-to-surface contact formulation. To validate the presented methodology, numerical examples in 3D are performed, including the contact patch test and Hertzian contact problem.

Numerically stable algorithm for an automatic detection and elimination of redundant nonlinear constraints and its embedding in the Lagrange multiplier, penalty, master-slave elimination methods

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Nonlinear multi-point constraints are used to model a wide range of features in engineering structures like incompressibility, inextensibility, rigidity or coupling of elements. The applied combination of such constraints can be either be non-redundant or redundant. There are three strategies to include nonlinear multi-point constraints in the finite element analysis: Lagrange multipliers, penalty method and master-slave elimination. Redundant nonlinear constraints are particularly challenging for all three methods. For Lagrange multipliers they can lead to a singular effective stiffness matrix and thus to divergence. For the penalty method redundancy worsens the convergence. For master-slave elimination redundant constraints lead to the selection of too many slave dofs or the wrong selection of master and slave dofs. This results in the failure of the method.

As the number of constraints in a given region of the system under study increases, the probability of the occurrence of redundant constraints also increases. For such problems it is not possible to detect the redundancy by hand because the coupling of constraints becomes very complex. An additional challenge is that the redundancy of constraints may change during the iterative solution process. Thus, redundant nonlinear constraints cannot be detected a priori in contrast to redundant linear constraints. Therefore, there is the need for an automatic detection and elimination of redundant nonlinear constraints during the simulation. However, in the literature redundancy has only been analyzed for certain combinations of constraints yet.

In this presentation we propose a direct, stable numerical method for the detection and elimination of arbitrary redundant nonlinear multi-point constraints that can be used for all three strategies. The corresponding treatment of the constraints has to be applied in each iteration. Thus, the presented method ensures the consistent linearization of the constraint forces and quadratic convergence is retained. We explain the algorithmic consequences on the three strategies due to the proposed method. In particular, we discuss the benefits of the method for the master-slave elimination as it gives also an automatic selection of master and slave dofs. We verify the method by selected examples and illustrate its influence on the numerical performance.

Robust optimization of truss structures considering uncertainties of 3D-printed continuous fiber composites

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Additive manufacturing enables the fabrication of geometrically complex structures, giving rise to a research focus on tailoring structures and material properties using numerical simulation. In lightweight engineering, continuous fiber composites are in great demand due to their superior strength-to-weight ratio. However, their anisotropic material properties pose difficulties for additive manufacturing processes: Planar 3D printing restricts fiber placement to a 2D plane, limiting the complexity of fabricated parts; current design methods for non-planar 3D printing (e.g., robotic arm) lack automated design methods with a performant integration of numerical simulation.

Another well-known problem of 3D-printed fiber composites is uncertainties in material parameters. Improvements in the micro-structure have been shown through consolidation or post-treatment (heat/pressure), reducing material variability. However, these methods are challenging to apply in non-planar 3D printing. Another approach is the experimental quantification of uncertainties in the material to incorporate them into the numerical simulation.

With the aim to contribute to design optimization for non-planar 3D printing of fiber composites, we develop a robust optimization methodology that considers firstly, the anisotropic nature of fiber composites and secondly, material uncertainties. The method is based on a ground structure discretization of the design space with 1D elements. It uses a heuristic approach for design optimization based on an optimality criteria for robustness aiming for equal strain energy distribution in the structure. The optimization methodology further utilizes the Certain Generalized Stresses Method (CGSM) for stochastic modeling to study the influence of the material uncertainties on the structural design.

List of Posters

Physiological Hill-type spindle model

Santana Chacon, Pablo Filipe (1); Hammer, Maria (1,2); Wochner, Isabell (1,2); Schmitt, Syn (1,2)

Po

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System optimization of multi-span beams through deformation adaptation

Schwegmann, Lisa

Po

University Rostock, Germany

On the numerical analysis of macro- and microscopic residual stresses in 3D

Hellebrand, Sonja; Brands, Dominik; Schröder, Jörg

Po

University of Duisburg-Essen, Germany

A numerical study on $Nd_2Fe_{14}B$ magnets produced by severe plastic deformation

Reichel, Maximilian; Schröder, Jörg

Po

University of Duisburg-Essen, Germany

Modeling of polycrystalline materials using a two-scale FE-FFT-based simulation approach

Schmidt, Annika; Gierden, Christian; Waimann, Johanna; Reese, Stefanie

Po

RWTH Aachen University, Germany

Physics informed neural networks for structural degradation modeling

Jilke, Lukas

Po

German Aerospace Center (DLR) / RWTH, Germany

Investigation of the role of the barrier parameter for the infeasible primal-dual interior point method for single crystal plasticity

Steinmetz, Felix; Scheunemann, Lisa

Po

RPTU Kaiserslautern-Landau, Germany

A nonlinear reduced order modelling approach to solid mechanics with application to representative volume elements

Faust, Erik; Scheunemann, Lisa

Po

RPTU Kaiserslautern-Landau, Germany

Finite element and isogeometric stabilized methods for the advection-diffusion-reaction equation

Key, Konstantin (1,3); Baidoo, Frimpong A. (2); Abdelmalik, Michael R.A. (4,2); Hughes, Thomas J.R. (2); Elgeti, Stefanie (3,1)

Po

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Attractors in the dynamics of large scale circulation in highly turbulent Rayleigh-Benard convection studied by the HAVOK method

Kašný, Jakub; Macek, Michal

Po

Czech Academy of Sciences, Czech Republic

Development of 3D printed adaptive structures for lower limb prostheses shafts

Ali, Ahmed Mohamed Jubartalla (1,2); Gfoehler, Margit (2); Riemelmoser, Franz (1); Kapl, Mario (1); Brandstötter, Mathias (1)

Po

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Modelling of interdependencies in process chains for cold-worked steel components

Furlan, Tim (1); Schewe, Markus (1); Menzel, Andreas (1,2)

Po

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