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# Prandtl Memorial Lecture and Plenary Lectures

**PML: Transition to the ultimate regime in Rayleigh-Bénard turbulence and other wall-bounded turbulent flows**

Speaker: **Lohse, Detlef** ***(University of Twente, Netherlands, The)***
Date: March 16, 2026 14:00–15:00
Room: KII, M17.01
Laudation: Hornung, Hans

In this talk I will reconcile the various experimental results on high-Rayleigh number Rayleigh-Benard (RB) turbulence. In this so-called ultimate turbulence regime, the Nusselt number (the dimensionless heat flux) has a steeper dependence on the Rayleigh number (the dimensionless temperature difference between top and bottom plate) than $Nu\,Ra^{1/3}$. The reason lies in the transition of a laminar type boundary-layer to a turbulent-type boundary layer. The transition is of non-normal-nonlinear nature, accounting for the large variation of observed transition Rayleigh numbers. We will also over a profound understanding of the heat transfer as function of the Rayleigh number and the Prandtl number of many decades in parameter space in both directions.

**PL1: From Models to Twins: Parametric Reduction for Adaptive Intelligence**

Speaker: **Chatzi, Eleni** ***(ETH Zürich, Switzerland)***
Date: March 16, 2026 15:00–16:00
Room: KII, M17.01
Chair: Steeb, Holger

Modern engineered systems are increasingly endowed with dense sensing, connectivity, and computational capabilities, giving rise to cyber-physical infrastructures and the notion of digital twins. While the resulting data richness creates unprecedented opportunities for monitoring, forecasting, and control, purely data-driven approaches often struggle to cope with the complexity, uncertainty, and high dimensionality inherent in real-world dynamical systems. In parallel, high-fidelity physics-based models remain computationally prohibitive and difficult to adapt online as systems evolve.
This lecture presents an integrative framework that bridges first-principles modeling and learning-based inference through parametric and representational reduction. Central to this approach is the construction of low-dimensional latent representations that preserve the essential dynamics and governing structure of complex systems, while enabling efficient simulation, identification, and adaptation. We discuss how physics-enhanced machine learning, structured architectures, and formal grammars can be combined to encode prior knowledge, enforce physical consistency, and promote interpretability and generalization.

**PL2: Modeling Damage with Nonlocal Approaches for Mesh-Objectivity - Time to Relax?**

Speaker: **Balzani, Daniel** ***(Ruhr-Universität Bochum, Germany)***
Date: March 17, 2026 11:00–12:00
Room: KII, M17.01
Chair: Schröder, Jörg

Computational modeling of damage progression is important for a variety of applications in civil and mechanical engineering, as well as biomedical applications. For example, estimating product lifespans requires the simulation of wear phenomena dominated by subcritical crack propagation under cyclic loading. Reusing reinforced concrete elements extracted from existing buildings relies on predicting future load-bearing capacities under pre-damaged material conditions. In the medical treatment of atherosclerotic arteries, computationally assisted estimation of plaque rupture probabilities helps to improve treatment while reducing costs. Therefore, the stress- and strain-softening effects that precede a crack and influence its propagation must be accurately described, e.g., using a constitutive continuum damage mechanical model. However, directly applying such models can create mesh dependencies in numerical simulations rendering the results uninterpretable. Several approaches are available to overcome this issue, including nonlocal integral-based models, gradient-enhanced formulations, and Eigenerosion schemes. These approaches come with additional length-scale-related parameters whose physical interpretation is still under investigation. An alternative, local approach is based on convexifying the associated incremental variational problem. This presentation will discuss recent progress on these approaches using numerical examples for different application problems.

**PL3: Analysis of the Multi-Dimensional Generalization of the Aw–Rascle Model**

Speaker: **Zatorska, Ewelina** ***(University of Warwick,)***
Date: March 17, 2026 12:00–13:00
Room: KII, M17.01
Chair: Lienstromberg, Christina

In this talk, I will discuss a multi-dimensional generalization of the well-known Aw–Rascle model for one-lane vehicular traffic. In the classical setting, the offset between the actual and desired velocities is described by a scalar function of the vehicle density. In higher dimensions, however, this offset can be naturally extended to the gradient of such a function. The function itself may incorporate both local and nonlocal effects, making the resulting model closely related to well-known systems in fluid mechanics, such as the degenerate viscosity compressible Navier–Stokes equations and the Euler–alignment equations used to describe collective motion.
I will first outline these connections at a formal level and highlight other contexts in which two-velocity formulations of hydrodynamic equations arise. I will then present several results concerning the existence of solutions in various frameworks—strong, weak, and measure-valued—and introduce analytical tools, such as relative entropy functionals, used to compare them. Finally, I will discuss derivations of these models from particle systems, their connections with kinetic descriptions, and several open problems in this area.

**PL4: Large-scale Bayesian inversion with complex models**

Speaker: **Petra, Noémi** ***(UC Merced, United States of America)***
Date: March 19, 2026 11:00–12:00
Room: KII, M17.01
Chair: Barth, Andrea

Model-based projections of complex systems will play a central role in prediction and decision-making. However, models are typically subject to uncertainties stemming from uncertain inputs in the model such as coefficient fields, source terms, etc. Refining our understanding of such models requires solving an inverse problem that integrates measurement data and the model to estimate and quantify the uncertainties in the parameters. Such problems face several challenges, e.g., high

dimensionality of the inversion parameters, expensive to evaluate models, constraints, and various sources of uncertainties. In this talk, we will focus on identifying and exploiting low-dimensional structure in such inverse problems stemming for example from local sensitivity of the data with respect to parameters, diffusive models, sparse data, etc. The key idea is to exploit the fact that we can access second derivative information (via Hessian-applies which translate to PDE solves), an operator that often exhibits a low rank and even a lower off-diagonal structure. We can leverage this structure to build efficient preconditioners for the Newton-Krylov systems, to reduce the parameter and state dimensions, and to build fast-to-evaluate proposals in an MCMC context. We present numerical results for an inverse problem governed by an ice sheet flow model.

## PL5: The Power that Binds Us: Computational Biomechanics in the Heart

Speaker: **Nordsletten, David** *(University of Michigan, United States of America)*
Date: March 19, 2026 12:00–13:00
Room: KII, M17.01
Chair: Röhrle, Oliver

Desmoplakin Cardiomyopathy (DSP-CM) is a genetic condition resulting from abnormal variants of the desmoplakin protein – a primary component of the complex linking sarcomeres across cell-cell junctions. DSP-CM leads to the progressive deterioration of cardiac muscle, developing subepicardial fibrosis that spreads around the heart. While the genetics of DSP-CM are known, the cause of this phenotype, disease progression, and how progression can be mitigated are not well known. However, adverse myocardial mechanics, forming elevated stresses manifesting into progressive cell damage and fibrotic remodeling presents a potential explanation to this observed pathophysiological phenomena.

To examine this theory, we look to understand the biomechanics of the heart, which relies on a hierarchical anisotropic nonlinear passive response to effectively promote filling and contraction of heart chambers and deliver blood flow throughout the body. This mechanical function exhibits fractional viscoelasticity, showing a power-law distribution of relaxation and rate dependent effects. Utilizing this understanding, we examine (N=29) patient-specific DSP-CM models at varying stages in the time course of their disease. Patient images were used to create patient-specific models and study the passive and active stresses, with specific emphasis on the subepicardium. Diseased myocardium was also studied in baseline and genetically modified induced pluripotent stem cell (iPSC) cardiomyocytes, formed into tissues and stressed for 48hrs.

Both scales highlight the potential importance of cardiomyocyte power to the progressive deterioration of heart muscle in DSP-CM. At the whole-organ level, image analysis and universal ventricular coordinates highlight the common patterns of disease, which are examined for mechanical variables, highlighting the importance of stress and strain-rate in these areas. At the the tissue scale, physiologically induced stress drives deterioration of DSP genetic variants, further accentuating the impact of power as a driving mechanism of cardiomyocyte damage. However, new results add a wrinkle to the story – accentuating the importance of viscoelastic biomechanics and mechanobiology to the mechanics of the heart.

Our results highlight the potential of cardiac biomechanics to elucidate the unique mechanics of the heart in disease – and the critical importance of understanding the mechanobiology of the heart. We demonstrate that DSP-CM shows progressive fibrosis that mirrors mechanics, providing potential clues to underlying drivers of damage and progressive fibrotic remodeling.

## PL6: Digital Twins in Materials Mechanics: From Descriptive to Predictive Models

Speaker: **Schulz, Katrin** *(Karlsruhe Institute of Technology,)*
Date: March 19, 2026 16:30–17:30
Room: KII, M17.01
Chair: Bischoff, Manfred

The transition from descriptive to predictive modeling of materials remains a key challenge in materials mechanics, particularly for crystalline materials whose macroscopic behavior emerges from complex interactions across multiple length and time scales. The talk presents a bottom-up perspective

on digital material twins, emphasizing the transition from descriptive to predictive models grounded in physical principles. Starting from classical crystal plasticity, the talk highlights how microstructural mechanisms such as dislocation activity, grain interactions, and phase morphology can be systematically incorporated into hierarchical modeling frameworks. While physics-based approaches provide interpretability and extrapolation capability, they are increasingly complemented by data-driven methods that enable the efficient exploitation of high-dimensional experimental and simulation data. Here, we focus on interpretable machine learning strategies tailored for materials mechanics. These include graph-based representations of microstructures, image-based analysis of evolving material states, and the emerging role of large
language models for knowledge extraction, model steering, and hybrid physics–data integration. Rather than replacing physical models, these approaches are discussed as enablers for enhanced model reliability, uncertainty quantification, and mechanistic insight. The presented concepts are illustrated through application examples in tribology and additive manufacturing, where strong process–structure–property relationships demand robust predictive capabilities. The lecture concludes by outlining key challenges and opportunities in developing digital material data twins that combine physical approaches with data-driven adaptability, paving the way towards predictive materials modeling.

## PL7: When PDE-constrained optimization becomes nonsmooth — and how we treat it

Speaker: **Ulbrich, Michael** *(Technische Universität München, Germany)*
Date: March 20, 2026 11:00–12:00
Room: KII, M17.01
Chair: Hahn, Bernadette

Nonsmoothness is a ubiquitous feature of modern optimization. It may be introduced deliberately as a modeling tool to promote specific solution structures, may emerge when inequalities or inclusions are reformulated as equations, or appear implicitly through solution operators of inclusions or constrained variational systems. Furthermore, risk-averse modeling leads to min-max formulations or nonsmooth risk measures. These challenges are amplified in the infinite-dimensional setting of PDE-constrained optimization, often making finite-dimensional techniques insufficient.

In this talk, we discuss key sources of nonsmoothness in PDE-constrained optimization, classify them according to where they enter the problem formulation, and present theoretical and algorithmic techniques for their treatment. The choice of appropriate methods depends crucially on whether nonsmoothness appears in the objective, the constraints, or in optimality conditions. For problems leading to nonsmooth systems of equations, we focus on Newton differentiability and semismooth Newton methods, a highly efficient class of superlinearly convergent algorithms. For problems with nonsmooth objective function, we discuss selected approaches that address nonsmoothness either directly or by smoothing strategies that integrate consistently with optimization algorithms. We also present several illustrating numerical examples.

## PL8: The Solver Bottleneck: Past, Present, and Future of Scalable Solvers for High-Order Methods

Speaker: **Persson, Per-Olof** *(UC Berkeley, United States of America)*
Date: March 20, 2026 12:00–13:00
Room: KII, M17.01
Chair: Stamm, Benjamin

High-order methods, such as Discontinuous Galerkin (DG) and Spectral Element Methods, offer exceptional accuracy for complex PDEs but create a significant "solver bottleneck." Due to the massive scale of the resulting algebraic systems, explicit methods have become popular. However, they often become intractable for real-world problems where stiff physics, poor element quality, stretched

meshes, or steady-state requirements lead to severe ill-conditioning. This necessitates the development of robust implicit strategies and iterative solvers that are scalable with respect to both problem size (h) and polynomial order (p).

We begin by reviewing foundational iterative strategies, tracing the evolution from block-Jacobi and p-multigrid preconditioned GMRES to ILU factorizations based on optimal element orderings (Minimum Discarded Fill). To exploit the benefits of efficient discretizations like DG-SEM and Line-DG on modern GPU architectures, purely matrix-free preconditioning is essential. This requirement motivated our work on Kronecker-structured SVD (KSVD) tensor approximations to represent dense elemental operators in a compressed, matrix-free format.

Building on this, the second half of the talk will focus on recent developments and current research. We will explore the design of robust and scalable multigrid methods, including agglomerated h-multigrid for handling complex geometries on unstructured meshes and adaptive smoothed aggregation (SA) multigrid, which has shown particular promise for DG and convection-dominated problems. We will also show how to incorporate static condensation into standard DG methods, allowing for a drastic reduction in problem size via a simple preliminary elimination step.

# Minisymposia and Young Researchers Minisymposia

## MS1: Large-Scale Bayesian Inference with a Machine Learning Twist

Organizer(s): de Wiljes, Jana *(TU Ilmenau)*
Roininen, Lassi *(LUT University)*

## MS1: Large-Scale Bayesian Inference with a Machine Learning Twist

Date: March 17, 2026 14:00–16:00
Room: KI, M11.32

### On the Algorithmic and Theoretical Path Towards Optimal Personalised Treatment

Hickl, Lisa (1); Hastermann, Gottfried (1); de Wiljes, Jana (1,2)
*1: Institute for Mathematics, Ilmenau University of Technology, Germany*
*2: School of Engineering Sciences, LUT University, Finland*

14:00

Tailoring medical treatment strategies to the covariates of specific patient subgroups or even to individuals has shown highly promising results in improving therapeutic outcomes. To enable personalized therapeutic approaches, a first essential step is to identify or learn the causal relationships between medical interventions, patient covariates and disease progression or improvement.
We illustrate this using a real-world data challenge on cellular information retrieval. Machine-learning methods such as Random Forests can provide deeper insights into potentially relevant biomarkers that distinguish healthy from diseased groups. In the context of rare immune disorders, such methods allow hidden relationships to be uncovered in a significantly shorter time frame compared to manual analysis.
Because the data is usually collected across multiple days, transport mapping is required to appropriately normalize the distributions to ensure technical variation does not interfere with patient-specific individuality. We further investigate under which mathematical conditions this transformation is justified. Once these relationships are established and a predictive model has been constructed, sequentially incoming patient data can be integrated with model predictions. This enables the use of reinforcement-learning techniques for optimal decision-making in the presence of uncertainty.

### Transporting Samples: ODE Flows, Importance Weights, and Higher-Order Methods

Klebanov, Ilja
*Freie Universität Berlin, Germany*

14:30

In this talk, we construct an ordinary differential equation with a closed-form right-hand side that transports a given probability distribution to a weighted mixture of its affine transformations. As a particular case, this yields an explicit transport map from a standard Gaussian to an arbitrary Gaussian mixture. This construction allows any quadrature rule — including quasi–Monte Carlo methods and sparse grids — to be transported from a simple reference distribution to the mixture, thereby significantly extending the applicability of higher–order sampling methods beyond classical settings.

We then discuss an appealing application to the Ensemble Kalman Filter (EnKF), which effectively samples from a Gaussian mixture at each update step. The transport framework enables the use of deterministic point sets in place of random ensembles, while consistency can be restored through several importance reweighting schemes.

**Efficient Amortized Bayesian Inference for Markov Random Fields via Gradient-Informed Grid Selection**

Bazahica, Laura (1); Avalos-Pacheco, Alejandra (2); Moores, Matthew (1); Roininen, Lassi (1)
*1: LUT University*
*2: JKU Linz*

15:00

Bayesian inference for models with intractable likelihoods, such as Markov random fields, requires a careful tradeoff between accuracy and computational cost. Various MCMC methods have been developed to address this challenge. The exchange algorithm targets the exact posterior, but relies on an expensive perfect sampling step at each iteration, which is often infeasible. In contrast, path sampling approximates the Metropolis acceptance ratio using a precomputed grid of likelihood values, but poorly chosen grids can introduce bias. Our approach builds on the theoretically robust framework of amortized inference for MCMC, providing accuracy comparable with the exchange algorithm, while substantially reducing the computational cost. We propose an efficient, gradient-informed method for selecting the precomputed grid. Hermite interpolation between these grid points results in a surrogate model that is easy to estimate with minimal approximation error. The advantages of our method are demonstrated by applications to a hidden Potts model of satellite data and an autologistic model of Arctic ice floes. A simulation study further quantifies the rate of improvement in accuracy as the number of grid points increases.

**Physics-Constrained Fine-Tuning of Flow-Matching Models for Generation and Inverse Problems**

Vollmer, Sebastian
*RPTU*

15:30

We present a framework for fine-tuning flow-matching generative models to enforce physical constraints and solve inverse problems in scientific systems. Starting from a model trained on low-fidelity or observational data, we apply a differentiable post-training procedure that minimizes weak-form residuals of governing partial differential equations (PDEs), promoting physical consistency and adherence to boundary conditions without distorting the underlying learned distribution. To infer unknown physical inputs, such as source terms, material parameters, or boundary data, we augment the generative process with a learnable latent parameter predictor and propose a joint optimization strategy. The resulting model produces physically valid field solutions alongside plausible estimates of hidden parameters, effectively addressing ill-posed inverse problems in a data-driven yet physics-aware manner. We validate our method on canonical PDE benchmarks, demonstrating improved satisfaction of PDE constraints and accurate recovery of latent coefficients. Our approach bridges generative modelling and scientific inference, opening new avenues for simulation-augmented discovery and data-efficient modelling of physical systems.

## MS2: Dynamics out of equilibrium

Organizer(s): Dall'Acqua, Anna *(Ulm University)*

### MS2: Dynamics out of equilibrium

Date: March 17, 2026 14:00–16:00
Room: KI, M11.42

**Gradient flows on metric graphs with reservoirs: Microscopic derivation and multiscale limits**

Heinze, Georg (1); Pietschmann, Jan-Frederik (2); Schlichting, André (3)
*1: WIAS Berlin, Germany*
*2: University of Augsburg, Germany*
*3: Ulm University, Germany*

14:00

In this talk, we will discuss evolution equations on metric graphs with reservoirs, that is graphs where a one-dimensional interval is associated to each edge and, in addition, the vertices are able to store and exchange mass with these intervals. Focusing on the case where the dynamics are driven by an entropy functional defined both on the metric edges and vertices, we provide a rigorous understanding of such systems of coupled ordinary and partial differential equations as (generalized) gradient flows in continuity equation format. Approximating the edges by a sequence of vertices, which yields a fully discrete system, we are able to establish existence of solutions in this formalism. Furthermore, we study several scaling limits using the recently developed framework of EDP convergence with embeddings to rigorously show convergence to gradient flows on reduced metric and combinatorial graphs. Numerical studies confirm our theoretical findings and provide additional insights into the dynamics under rescaling. Finally, we highlight possible extensions towards models with multiple layers.
Based on joint work with Jan-Frederik Pietschmann and André Schlichting.

**On the derivation of multiscale ferrofluid models**

Girodroux-Lavigne, Alexandre; Höfer, Richard
*Universität Regensburg, Germany*

14:20

We consider a microscopic model of N magnetic nanoparticles in a Stokes flow.
We assume that the temperature is above the critical Néel temperature such that the particles' magnetizations undergo random flip with rate $1/\varepsilon$. The microscopic system is the modeled through a piecewise deterministic Markov jump process. We show that for large N , small particle volume fraction and small $\varepsilon$, the system can be effectively described by a multiscale ferrofluid model.

**The direction energy method in non-compact mean curvature flow**

Rupp, Fabian (1); Miura, Tatsuya (2)
*1: University of Vienna, Austria*
*2: Kyoto University, Japan*

14:40

Mean curvature flow is classically understood as the $L^2$-gradient flow of the volume functional. In the non-compact setting, however, this variational interpretation degenerates, since the volume is infinite and the associated energy identity becomes vacuous. In this talk, we present a new variational framework for non-compact mean curvature flow by interpreting it as the gradient flow of a direction energy. Although this functional differs from the volume by a formal null-Lagrangian, it can be finite for non-compact hypersurfaces, and enables us to study the behavior of global solutions.

**Co-Moving Volumes and the Reynolds Transport Theorem for Two-Phase Flows**

Bothe, Dieter (1); Köhne, Matthias (2)
*1: TU Darmstadt, Germany*
*2: HHU Düsseldorf, Germany*

15:00

We consider the local kinematics at fluid interfaces in two-phase flows within the sharp interface framework. In the considered case with phase change and slip at the interface, the governing velocity field is discontinuous at the phase boundary with possible jumps of the normal and the tangential components. This causes the associated initial value problems for the kinematic differential equation, governing the motion of fluid elements, to be ill-posed in general. Motivated by a corresponding example, where the velocity field is physically consistent regarding the balance of mass and momentum as well as the entropy inequality, we employ concepts from differential inclusions, to rigorously define co-moving sets within this framework. The main point of the talk then is to explain how an extended version of the Reynold transport theorem can be obtained for such general two-phase flows.

**Mean-Field Limit and fluctuation for systems with singular interaction**

Chen, Li
*Universität Mannheim, Germany*

15:20

Mean-field limit and a central limit theorem is shown for moderately interacting particles in the whole space. The interaction potential approximates singular attractive or repulsive potentials of sub-Coulomb type. The fluctuation around the mean field limit is shown to become asymptotically Gaussians. The key step in the rigorous proof is the mean-square convergence in expectation for smoothed empirical measures associated to moderately interacting N-particle systems with rate N-1/2-$\varepsilon$for some $\varepsilon$> 0. The talk is given based on a joint work with Alexandra Holzinger and Ansgar Jüngel.

**Hypocoercivity of non-equilibrium steady states (in kinetic theory)**

Dietert, Helge
*CNRS, Paris Cité, France*

15:40

In kinetic theory, we have densities over the phase space of position x and velocity v. The collision operator creating dissipativity only acts on the velocity and hypocoercivity describes the combination with the transport operator to create global coercivity. In this talk, I will present how hypocoercivity can be understood in the non-equilibrium setting.

## MS3: Advances in the Numerical Treatment of Quantum Systems

Organizer(s): Altmann, Robert *(OvGU Magdeburg)*
Henning, Patrick *(Ruhr University Bochum)*

## MS3: Advances in the Numerical Treatment of Quantum Systems

Date: March 17, 2026 14:00–16:00
Room: KI, M11.62
Chair(s): Henning, Patrick

### Riemannian optimization for multicomponent Bose-Einstein condensates: algorithms and convergence analysis

Altmann, Robert (1); Hermann, Martin (2); Peterseim, Daniel (2); Stykel, Tatjana (2); Yadav, Mahima (3)
*1: Otto-von-Guericke-Universität Magdeburg*
*2: Universität Augsburg*
*3: Ruhr-Universität Bochum*

14:00

In this talk, we address the computation of ground states of multicomponent Bose-Einstein condensates in both non-rotating and rotating regimes. These states can be characterized either as minimizers of a constrained energy functional or as solutions to a coupled nonlinear Gross-Pitaevskii eigenvalue problem, where the nonlinearity arise from inter-component interactions. For solving these problems, we adopt a Riemannian optimization approach that exploits the intrinsic geometric structure of the constraint manifold induced by mass conservation laws. To resolve the non-uniqueness of ground states of rotating condensates caused by phase symmetry, we formulate the minimization problem on an appropriate quotient manifold. Endowing this manifold with a general Riemannian metric, we present a Riemannian gradient descent method and analyze its local convergence by deriving explicit convergence rates under suitable assumptions on the physical model and the chosen metric. Specializing this framework to energy-adaptive and Lagrangian-based metrics, tailored to the energy and constraints landscape, we construct preconditioned Riemannian optimization schemes with enhanced convergence properties. Numerical experiments demonstrate the computational efficiency of the proposed algorithms.

### Self-consistent field iterations in electronic structure

Levitt, Antoine
*Université Paris-Saclay, France*

14:30

I will report on recent work on numerical methods for solving the self-consistent problem in electronic structure.

### Learning the density matrix of Kohn-Sham Density Functional Theory - towards a foundational model

Zhang, Liwei (1); Mazzeo, Patrizia (2); Nottoli, Michele (3); Cignoni, Edoardo (2); Cupellini, Lorenzo (2); Stamm, Benjamin (1)
*1: RWTH Aachen University*
*2: Università di Pisa*
*3: University of Stuttgart, Germany*

15:00

This talk begins with a concise introduction to Kohn–Sham Density Functional Theory (KS-DFT) as a framework for modeling the behavior of electrons in the presence of nuclei at fixed positions. The associated solution operator maps the nuclear coordinates to the central unknown of KS-DFT, namely the electronic density matrix (DM). We discuss the invariance and equivariance properties of the density matrix with respect to nuclear coordinates and introduce a framework for representing the DM as a function of these coordinates using the Atomic Cluster Expansion (ACE). This representation enables the construction of a learning strategy for the solution map. The talk concludes with numerical

examples demonstrating the systematic improvability of the approach, as well as a discussion of its current limitations and future perspectives.

**A geometric interpretation of (quantum) optimal transport**

Borsoni, Thomas (1); Dusson, Geneviève (2); Ehrlacher, Virginie (1)
*1: Ecole Nationale des Ponts et Chaussées, France*
*2: Université Bourgogne Franche-Comté*

15:30

Quantum optimal transport aims at defining distances and interpolations between density matrices, viewed as quantum analogues of probability measures in classical optimal transport. In this work, we discuss a geometric interpretation of Kantorovich-type formulations of optimal transport, as an extension of a cost from the set of extreme points of a convex to the entire convex. We show that this framework encompasses both the classical case, when the convex is a simplex, and the quantum case without entanglement.

## MS4: Operator Learning and Continuous Numerical Linear Algebra

Organizer(s): Kressner, Daniel *(EPFL)*
Colbrook, Matthew *(University of Cambridge)*

## MS4: Operator Learning and Continuous Numerical Linear Algebra

Date: March 17, 2026 14:00–16:00
Room: KII, M17.01

### Koopman operator learning: error bounds and closed-loop control with guarantees

Bold, Lea (1); Hertel, Maximiliano (1); Philipp, Friedrich M. (1); Schaller, Manuel (2); Worthmann, Karl (1)
*1: Technische Universität Ilmenau, Germany*
*2: Technische Universität Chemnitz, Germany*

14:00

Extended dynamic mode decomposition, embedded in the Koopman framework [4], is a widely applied technique to predict the evolution of an observable function along the flow of dynamical systems. However, despite its popularity, the error analysis is still fragmentary. We provide an analysis of the full approximation error [3,2] including an extension to control systems [1]. To this end, we show Koopman invariance of suitably-constructed reproducing kernel Hilbert spaces (RKHS) and leverage approximation-theoretic arguments for (regularised) kernel EDMD. Then, we extend the results to control affine systems and demonstrate the applicability of the data-driven Koopman surrogate model for model predictive control [5], see also the recent overview paper [7].

**References**:

[1] L. Bold, F.M. Philipp, M. Schaller, and K. Worthmann: Kernel-based Koopman approximants for control: Flexible sampling, error analysis, and stability. **SIAM Journal on Control and Optimization** 63(6):3825-4114, 2025

[2] M. Hertel, F.M. Philipp, M. Schaller, and K. Worthmann: Koopman for stochastic dynamics: error bounds for kernel extended dynamic mode decomposition, arXiv preprint https://arxiv.org/abs/2512.20247

[3] F. Köhne, F.M. Philipp, M. Schaller, A. Schiela, and K. Worthmann. $L^\infty$-error bounds for approximations of the Koopman operator by kernel extended dynamic mode decomposition. **SIAM Journal on Applied Dynamical Systems** 24(1):501–529, 2025

[4] I. Mezic. Spectral properties of dynamical systems, model reduction and decompositions. **Nonlinear Dynamics** 41:309–325, 2005

[5] I. Schimperna, K. Worthmann, M. Schaller, L. Bold, and L. Magni. Data-driven model predictive control: Asymptotic stability despite approximation errors exemplified in the Koopman framework, arXiv preprint arXiv:2505.05951

[7] R. Strässer, K. Worthmann, I. Mezic, J. Berberich, M. Schaller, and F. Allgöwer. An overview of Koopman-based control: From error bounds to closed-loop guarantees. **Annual Reviews in Control** 61:101035, 2026

### Koopman-Schur decomposition for learning nonlinear dynamics

Drmac, Zlatko (1); Mezic, Igor (2)
*1: Faculty of Science, University of Zagreb, Croatia*
*2: Department of Mechanical Engineering, University of California at Santa Barbara*

14:20

The Dynamic Mode Decomposition (DMD) is a popular and versatile numerical method for data driven analysis of nonlinear dynamical systems. The theoretical bedrock upon which the more general Extended DMD framework (EDMD) is built is the Koopman composition operator.
EDMD can be described as data driven Rayleigh-Ritz extraction of spectral information of the Koopman composition operator associated with the underlying dynamical system. The nonlinear data snapshots are represented using the eigenvectors/eigenfunctions of the operator, resulting in a

modal (spatio-temporal) decomposition KMD (Koopman Mode Decomposition) of the data snapshots. The KMD can be considered as a model order reduction tool that represents the nonlinear dynamics using selected eigenpairs of the operator which is in fact an infinite dimensional linearisation of the nonlinear dynamics. It can be used to reveal coherent states and for forecasting and control. In some cases, numerically computed compression of the Koopman operator exhibits high non-normality, and, as a result, the eigenvectors are highly ill-conditioned and the KMD becomes numerically unstable. This depends on the operator and on the basis (functions) used to derive finite dimensional compression.
We present recently introduced theoretical and computational framework for data driven Koopman modal analysis, which mitigates the problem of ill-conditioned eigenvectors. It uses a Schur decomposition of the Koopman operator, entirely based on unitary transformations. The analysis in terms of the eigenvectors as modes of a Koopman operator is replaced with a modal decomposition in terms of a flag of invariant subspaces that correspond to selected eigenvalues. All subspaces are parametrized using orthonormal bases.
The main computational tool from the numerical linear algebra is the partial ordered Schur decomposition, that provides orthonormal bases for invariant subspaces corresponding to selected eigenvalues. A reordering trick to construct invariant subspace for selected eigenvalues, and the kernel trick to allow for high dimensional embeddings can be used.

Further, for the Koopman operator defined on some classes of funcion spaces, we prove the existence of the Schur decomposition and the convergence of the numerical algorithm.

**Operator Learning for Hyperbolic PDEs and its Applications in Weather and Climate Prediction**

Bonev, Boris (1); Kurth, Thorsten (1); Mahesh, Ankur (2); Bisson, Mauro (1); Liu-Schiaffini, Miguel (3); Berner, Julius (1); Kossaifi, Jean (1); Kashinath, Karthik (1); Azizzadenesheli, Kamyar (1); Pritchard, Michael S. (1); Collins, William D. (2); Anandkumar, Anima (3); Keller, Alexander (1)
*1: NVIDIA Corporation, Santa Clara, CA 95051, United States*
*2: Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States*
*3: California Institute of Technology, Pasadena, CA 91125, United States*

14:40

Neural operators have emerged as powerful tools for learning solution operators of partial differential equations in a resolution-agnostic manner. However, standard Fourier Neural Operators (FNOs) face fundamental limitations when applied to spherical geometries, as the discrete Fourier transform assumes flat geometry, causing visual and spectral artifacts and pronounced dissipation in spherical coordinates. This talk presents our work on developing geometric operator learning methods that respect the inherent symmetries and topology of the sphere, with applications to the chaotic dynamics of Earth's atmosphere.

We implement two complementary approaches: group convolutions and attention mechanisms generalized to spherical geometry. The Spherical Fourier Neural Operator (SFNO) is formulated for spherical geometry through Driscoll-Healy's convolution theorem, which connects the Spherical Harmonic Transform (SHT) to group convolutions on the sphere. This approach provides theoretical guarantees of rotational equivariance while retaining grid-invariance, enabling stable autoregressive rollouts for a year of simulated time while maintaining physically plausible atmospheric dynamics.

While global spectral methods excel at capturing long-range dependencies, hyperbolic PDEs often exhibit local features and sharp gradients that require localized representations. We present a principled framework for incorporating localized integral and differential operators into neural operator architectures. Drawing inspiration from numerical methods for PDEs, we derive differential layers that provably converge to differential operators, and utilize quadrature rules to compute discrete-continuous convolutions that approximate local integral operators on both Euclidean and spherical geometries.

To complement convolutional approaches, we further develop a generalized attention mechanism for spherical domains that enables Transformer architectures to natively process data on the two-dimensional sphere. We derive a discretization-agnostic spherical attention operator by integrating

numerical quadrature weights into the continuous spherical formulation of the attention mechanism, obtaining geometrically faithful spherical attention that is approximately rotationally equivariant.

Finally, we demonstrate practical impact through FourCastNet 3, a scalable probabilistic weather forecasting system built as a hidden Markov model using spherical signal processing primitives. The system delivers forecasting accuracy surpassing leading conventional ensemble models and rivaling state-of-the-art diffusion methods, while producing forecasts 8 to 60 times faster. These innovations position geometric neural operators as robust foundations for next-generation weather and climate modeling systems.

**Randomized Nyström approximation of non-negative self-adjoint operators**

Persson, David (1); Boullé, Nicolas (2); Kressner, Daniel (3)

*1: New York University & Flatiron Institute, United States of America*
*2: Imperial College London, United Kingdom*
*3: EPFL, Switzerland*

15:00

The randomized singular value decomposition (SVD) has become a popular approach to computing cheap, yet accurate, low-rank approximations to matrices due to its efficiency and strong theoretical guarantees. Recent work by Boullé and Townsend (FoCM, 2023) presents an infinite-dimensional analog of the randomized SVD to approximate Hilbert-Schmidt operators. However, many applications involve computing low-rank approximations to symmetric positive semi-definite matrices. In this setting, it is well-established that the randomized Nyström approximation is usually preferred over the randomized SVD. This work explores an infinite-dimensional analog of the Nyström approximation to compute low-rank approximations to non-negative self-adjoint trace-class operators. We present an analysis of the method and, along the way, improve the existing infinite-dimensional bounds for the randomized SVD. Our analysis yields bounds on the expected value and tail bounds for the Nyström approximation error in the operator, trace, and Hilbert-Schmidt norms. Numerical experiments on integral operators arising from Gaussian process sampling and Bayesian inverse problems are used to validate the proposed infinite-dimensional Nyström algorithm.

**Rigorous Data-Driven Spectral Analysis of Nonlinear Dynamics**

Colbrook, Matthew (1); Boullé, Nicolas (2); Conradie, Gustav (1); Townsend, Alex (3)

*1: University of Cambridge, United Kingdom*
*2: Imperial College London, UK*
*3: Cornell University, USA*

15:20

We present a unifying framework for rigorous, data-driven spectral analysis of nonlinear dynamical systems using Koopman operator theory. While Koopman operators provide a global linear representation of nonlinear dynamics, their infinite-dimensional nature creates major computational challenges. We introduce provably convergent algorithms for computing Koopman spectral properties from snapshot data, including Residual Dynamic Mode Decomposition (ResDMD), which avoids spectral pollution and provides *a posteriori* error control for spectra, pseudospectra, and spectral measures—even in chaotic and high-dimensional systems. Building on this foundation, we introduce SpecRKHS, a kernel-based framework that defines Koopman operators on Reproducing Kernel Hilbert Spaces, enabling flexible function representations, pointwise prediction with error bounds, and efficient high-dimensional computation. Applications to turbulent flows, molecular dynamics, and climate data illustrate the practical power of these methods. If time permits, we will also discuss impossibility results that reveal fundamental limits of data-driven spectral learning.

**Rigorous Data-Driven Forecasts of Nonlinear Dynamics**

Conradie, Gustav (1); Boullé, Nicolas (2); Brunton, Steve (3); Colbrook, Matthew (1)

*1: University of Cambridge, United Kingdom*
*2: Imperial College London, UK*
*3: University of Washington, USA*

15:40

Koopman-based models lift nonlinear dynamics on a finite-dimensional state space to an infinite-dimensional function space, allowing for a global linearization of the dynamics. By considering the

functions which correspond to the state coordinates, we can use the Koopman operator to predict the original dynamics. However, when approximating the Koopman operator from data we can only learn it on a finite-dimensional function space, necessitating a limit to achieve convergence. While convergence of this limit is known, less studied is the rate of convergence, and in particular a posteriori error bounds, telling us how close our forecasts are to the true dynamics. In this talk we will discuss new algorithms which compute rigorous error bounds for the Koopman operator, both in the classical $L^2$ setting and the kernelized setting, which allows for pointwise rather than norm error bounds. We also introduce a framework for computing the expected errors in forecasts, as well as use techniques for measuring subspace invariance to produce a novel dimension reduction tool for Koopman operators. We will discuss applications to systems including cavity fluid flows and orbital dynamics.

## MS5: Experimental Solid Mechanics

Organizer(s): Kiefer, Björn *(TU Bergakademie Freiberg)*
Gerke, Steffen *(nan)*
Lehmann, Thomas *(Chemnitz University of Technology)*

## MS5: Experimental Solid Mechanics

Date: March 17, 2026 14:00–16:00
Room: KII, M17.02
Chair(s): Kiefer, Björn
Gerke, Steffen
Lehmann, Thomas

### Material Testing 2.0 for Plasticity Model Calibration: Progress, Challenges, and the Road Ahead

COPPIETERS, SAM (1); Maček, Andraž (2); Starman, Bojan (3); Halilovič, Miroslav (4) 14:00
*1: KU Leuven*
*2: KU Leuven*
*3: University of Ljubljana*
*4: University of Ljubljana*

This presentation provides a comprehensive overview of nearly a decade of research on Material Testing 2.0 (MT2.0) for the calibration of plasticity models. It begins by exploring the fundamental pillars of MT2.0 within a historical context, highlighting their conceptual evolution and established interconnections. The discussion then transitions to the current state-of-the-art in MT2.0 for metal plasticity, with the goal of drafting a clear roadmap for industrial valorization in the years ahead. While MT2.0 is widely recognized by leading industrial stakeholders as a transformative framework for developing interoperable digital tools that reduce experimental efforts in material model calibration, it faces a critical challenge: its reliance on integrating expertise from traditionally distinct disciplines. The final part of the presentation examines practical pathways for industrial adoption, emphasizing the development of integrated solutions that minimize the need for end-user expertise in the underlying pillars. These efforts aim to unlock the full potential of MT2.0, facilitating widespread implementation and maximizing its industrial impact.

### Energy absorption properties of different cellular materials

Weinberg, Kerstin 14:40
*University of Siegen, Germany*

Energy absorption under compressive load and impact is a key feature for the use of cellular materials in lightweight construction, protection, and damping applications. The design of the cellular microstructure is essential, as it influences the deformation behavior significantly.
For this reason, three structural classes of cellular materials are compared experimentally. While open-cell foams are characterized by a stochastically distributed cell geometry consisting of nodes and ligaments, beam-based lattice structures are composed of regular arrangements in unit cells. In contrast to both architectures, triply periodic minimal surfaces (TPMS) structures do not contain discrete nodes; they are formed by continuous, smooth, and periodic surfaces. To enable an objective comparison, open-cell foams, TPMS, and conventional beam-based lattice structures with identical relative density are manufactured and then experimentally examined under pressure loading.

### Coupled infrared thermography and digital image correlation - assessment of temperature gradient and temperature velocity

Tröger, Jendrik-Alexander; Müller-Lohse, Lutz; Hartmann, Stefan 15:00
*Clausthal University of Technology, Germany*

Full-field measurement methods have matured in recent years and are well established in experimental solid mechanics, providing extensive, information-rich datasets. Among the many available

techniques, digital image correlation is widely applied to analyze the surface deformation, often in a stereocorrelation-based setup employing two visible light cameras. If thermal effects are of interest, infrared thermography is used to quantify temperature fields on surfaces. Although both measurement techniques are frequently employed to provide data for model calibration and validation of numerical simulations, their coupling is not straightforward. It must be considered that infrared thermography provides data in an Eulerian setting, which contrasts with digital image correlation. As a remedy, a projection using a camera model is necessary to express both datasets in the same Lagrangian frame.

In this study, we investigate the coupling of two-dimensional temperature data measured by infrared thermography and three-dimensional point coordinates from stereocorrelation-based digital image correlation for the analysis of curved surfaces. Unlike existing multiview approaches, we utilize two independently calibrated industrial-grade systems. The projection matrix of the pinhole camera model is calibrated using a reference object. Through this projection, temperature and displacement fields are accurately represented at material points in the sense of continuum mechanics. This approach is particularly suited for, but not restricted to, curved surfaces. After both datasets are expressed in the same Lagrangian frame, we utilize radial basis functions to interpolate the point-wise data. This allows the computation of temperature gradients and temperature velocity, providing even more insights into the thermo-mechanical material behavior from full-field measurements.

**Crack paths in ferroelectrics: why established anisotropic deflection criteria have to fail**

Ricoeur, Andreas; Zarjov, Konstantin; Wang, Zhibin 15:20
*Universität Kassel, Institut für Mechanik, Germany*

Cracks are known to potentially deflect in solids with anisotropic fracture toughness, even under pure mode-I loading, which prevails, e.g., if tensile stress is applied perpendicular to a straight pre-crack. The prerequisite for this is that the degree of anisotropy, in terms of the ratio of the largest to smallest toughness, exceeds a threshold, which depends on the specific angular course of toughness and the deflection criterion. The latter can be stress-based or rely on the maximum release of potential energy. In any case, the threshold typically ranges between 1.2 and 1.5, which is confirmed by experiments, e.g., based on a forged aluminum alloy [1]. In piezo- or ferroelectrics, such as lead zirconate titanate or barium titanate, experiments with Vickers indentations reveal toughness ratios which are far beyond this threshold [2], which is identified based on the dissimilar lengths of perpendicular cracks, initiating from the corners of the indenter. Surprisingly, none of the cracks deflect in the experiments, which is contradictory to what is observed in anisotropic structural materials, and to predictions based on established anisotropic deflection criteria. Nevertheless, in all crack growth simulations of piezoelectrics, published to date, crack deflection is handled just as in structural materials, leading to moderate and even contradictory results, compared to recent three-point-bending experiments in PZT under electromechanical loading conditions [3]. These, by the way, differ significantly from acknowledged experimental findings in the 1990s [4], which, however, still serve as reference of simulations today. Obviously, ferroelectrics are subject to different rules in this respect, and crack deflection has to be modeled on another basis, where domain switching must not be neglected. In this paper, experimental findings of crack paths in structural materials and in piezoelectrics are compared, the cause of the fundamentally difference behaviors is being elucidated, and an appropriate deflection criterion is presented.

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**Experimental Investigation and Modification of Meta-Materials for Energy Absorption Applications**

Sharma, Prateek; Jung, Anne 15:40
*Helmut-Schmidt-Universität/ Universität der Bundeswehr, Hamburg, Germany*

Metamaterials show immense potential for energy absorption in applications such as protective equipment, crash absorbers, and blast protection due to their superior mechanical tunability and lightweight characteristics. This study presents an experimental investigation of different classes of metamaterials, including auxetic and triply periodic minimal surface (TPMS) structures, with the objective of evaluating their energy absorption performance under varying loading conditions.

Various specimens with different structural parameters such as cell size and relative density were 3D-printed from the photosensitive polymer BASF Ultracur3D® ST 1400 using stereolithography. Quasi-static compression tests were conducted to evaluate the deformation mechanisms and stress–strain response. To investigate the energy absorption capacity under dynamic loading, the structures were further tested at high strain rates using drop tower and dynamic compression experiments. In addition, the bulk material was characterized through tensile and compression tests at various strain rates.

Based on the results, material and structural effects were successfully isolated, enabling systematic modification of the architectures to achieve improved energy absorption capacity. The results demonstrate that structural topology plays a critical role in governing energy absorption behavior. Systematic variation of geometric parameters such as cell size, relative density, and topology enabled tailored mechanical responses for targeted energy absorption applications. Auxetic and TPMS-based architectures exhibited enhanced progressive collapse and delayed densification compared to the bulk material and conventional open-celled foams, leading to significantly improved energy absorption efficiency.

## YRM1: Mathematical Analysis of active cells

Organizer(s): Stephan, Artur *(Technische Universität Wien)*
Heinze, Georg *(WIAS Berlin)*

## YRM1: Mathematical Analysis of active cells

Date: March 16, 2026 16:30–18:30
Room: KI, M11.42

### Stability of equilibria of the spatially inhomogeneous Vicsek-BGK equation

Egger, Stefan (1); Kogelbauer, Florian (2)
*1: TU Wien, Austria*
*2: ETH Zürich, Switzerland*

16:30

We study the stability of equilibria in the Vicsek model. It is a mathematical model for a variety of physical phenomena, with collective motion and swarming among the most studied ones. Therefore, it has applications both on the macroscopic level (e.g., flocks of birds, crowds, or car traffic) and on the microscopic level (e.g., colonies of bacteria and cells). Swarming on the cellular level is an important factor when describing processes like wound healing, embryogenesis, or tumor cell invasion, which heavily depend on coordinated cellular motion.
The spatially homogeneous model exhibits a phase transition: For small particle density, there is a unique equilibrium, which corresponds to a completely unordered state. For high enough density, a bifurcation occurs, and a second branch of equilibria emerges, which corresponds to an ordered state with a dominant direction of alignment. In the spatially homogeneous setting, the equilibria and their stability are fully characterized; however, in the spatially inhomogeneous setting, little is known about the ordered equilibrium states emerging at high density. Doing a spectral analysis of the linearized system, we show that they get unstable for sufficiently large density, which is in stark contrast to the spatially homogeneous setting.

### Pattern selection in a mechanochemical model of pattern formation

Münnich, Finn (1); Cygan, Szymon (1); Oelz, Dietmar (2); Marciniak-Czochra, Anna (1)
*1: Heidelberg University, Germany*
*2: University of Queensland, Australia*

16:50

Hydra is renowned for its regenerative abilities and serves as a key model for studying body axis formation. Mechanical cues influence cell fate decisions during development and regeneration, yet the underlying mechanisms remain unclear. We propose a mechanochemical model for body axis formation in regenerating Hydra tissue spheroids, coupling morphogen dynamics to tissue mechanics through a positive feedback loop: mechanical stretching enhances morphogen production, while morphogen concentration modulates tissue elasticity. This feedback realizes a mechanochemical variant of the local activation–long range inhibition paradigm. Using a reduced one-dimensional model, we analyze patterns analytically. We prove the existence of stable non-constant steady states and show that all multimodal solutions are linearly unstable, implying that stable patterns are always unimodal. Our results indicate that mechanochemical coupling provides a robust mechanism for generating single-peaked patterns without a second diffusible inhibitor.

### Curvature-driven pattern formation in biomembranes: A gradient flow approach

Knopf, Patrik (2); Pešić, Anastasija (1); Trautwein, Dennis (2)
*1: WIAS Berlin*
*2: Universität Regensburg*

17:10

In this talk, we will present a phase-field model for curvature-driven pattern formation in biomembranes. The model is obtained as the gradient flow of an energy approximating the two-phase Canham–Helfrich functional, which leads to a Cahn–Hilliard-type equation with cross diffusion for the lipid concentration, coupled to a fourth-order equation governing the membrane height. We will outline the analytical framework establishing existence and uniqueness of weak solutions for both

regular and singular potentials. Additionally, numerical simulations will be presented illustrating how different parameter regimes produce striped, dotted, or snake-like membrane patterns. The talk is based on a joint work with Patrik Knopf and Dennis Trautwein.

**A free boundary problem modeling cell polarization**

Logioti, Anna (1); Niethammer, Barbara (2); Röger, Matthias (3); J. L. Velázquez, Juan (2)
*1: Universität Stuttgart, Germany*
*2: Universität Bonn, Germany*
*3: Technische Universität Dortmund, Germany*

17:30

We consider a model for cell polarization as a response to an external signal which consists of a bulk-surface reaction-diffusion system of equations. We study the evolution of this model in certain parameter regimes in which several reaction rates on the membrane as well as the diffusion coefficient within the cell are large. It turns out that, in suitable scaling limits, the system converges to a non-local free boundary problem. In this talk, I will present several results for this problem, starting with an L1-contraction property and, in the case of time-constant signals, the stability of stationary states. In addition, I will address some qualitative properties of the free boundary. More precisely, we have concluded that there are necessary and sufficient conditions for the initial data that yield continuity of the support at t=0. If one of these assumptions fail, then jumps of the support take place. We have further provided a complete characterization of the jumps for a large class of initial data.

**Critical lack of detailed balance in stochastic proofreading models**

Franco, Eugenia
*University of Bonn, Italy*

17:50

The detailed balance is a property of macroscopic systems that are obtained from an underlying time reversible microscopic model. It states that each elementary process (for instance each chemical reaction) is at equilibrium with its reverse process.
In this talk, I will discuss the role of the lack of detailed balance in a class of stochastic kinetic proofreading models. Kinetic proofreading systems were proposed by Hopfield and Ninio in the 70's in order to explain the way in which receptors can distinguish between different ligands with a low error rate. This ability is referred to as specificity.
We prove the existence of a critical amount of lack of detailed balance that kinetic proofreading models must have in order to have strong specificity.

**Living or non-living? Structural conditions for multi-scale reaction kinetics**

Spellmann, Holger; Schlichting, André
*Ulm University, Germany*

18:10

Living systems and cellular subsystems are driven by biochemical reaction networks operating out of thermodynamic equilibrium. A key open question is to identify structural criteria that distinguish such nonequilibrium networks from those that admit an equilibrium description. As a contribution to this problem, we analyze which reaction kinetics can arise as multi-scale limits of mass-action kinetics that satisfy detailed balance. We derive a necessary criterion for such effective kinetics, formulated as the existence of a discrete gradient field on the reaction graph governing the timescale order of the propensities. This condition can be viewed as a generalized Wegscheider condition for multi-scale limits. Furthermore, we relate our criterion to the notion of extended detailed balance at the microscopic level. This is joint work with André Schlichting.

## YRM2: Robust and Reliable Solution Techniques for Multiphysics in Porous Media

Organizer(s): Dağlı, Tugay *(TU Chemnitz)*
Brodbeck, Maximilian *(University of Stuttgart)*

## YRM2: Robust and Reliable Solution Techniques for Multiphysics in Porous Media

Date: March 16, 2026 16:30–18:30
Room: KI, M11.32
Chair(s): Dağlı, Tugay
Brodbeck, Maximilian

### Solvers for mixed finite element methods based on spanning trees

Boon, Wietse M. (1); Fumagalli, Alessio (2)
*1: University of Duisburg-Essen, Germany*
*2: Politecnico di Milano, Italy*

16:30

Mixed finite element methods are capable of respecting physical conservation laws at the discrete level, by preserving the structure of the governing PDEs. However, this often leads to computationally demanding saddle point systems with a large number of degrees of freedom. Robust and reliable solvers are therefore essential to make these methods feasible for large-scale problems.

In this talk, we consider a decomposition of conventional finite element spaces, based on spanning trees in the grid. With this decomposition, we form a new basis in which the mixed formulation of Darcy flow unravels from a large saddle-point problem into four smaller, symmetric positive definite systems. The resulting direct solver allows us to achieve a significant computational speed-up, without loss of accuracy.

We proceed by generalizing the solver to two related problems. First, we consider a model in which fractures are represented by subdomains of lower dimensionality. We show that the theory directly applies to this case and present similar computational gains. Finally, we show the extension to a mixed formulation of linearized elasticity, in which the stress is an explicit variable in the system. If time allows, we conclude with the implications for designing reliable neural network solvers that respect physical constraints.

### Time Parallel Vectorized Block Krylov Methods with applications to Porous Media problems

Schell, Alexander; Engwer, Christian; Dreier, Nils-Arne
*University of Münster, Germany*

17:10

Higher order methods are widely regarded as a promising way to overcome performance issues in simulations of partial differential equations (PDEs) on modern hardware. Nevertheless, many users stick to low-order, matrix-based simulations, in particular in porous media applications where heterogeneous coefficients and low regularity of the solution are reasons not to employ higher order discretizations.
In this talk we present a novel approach for the simulation of time-dependent PDEs that aims to partially mitigate the performance problems of classical time-stepping schemes. By reformulating the original problem we derive a parallel in time (PinT) time integrator that increases the arithmetic intensity and introduces additional structure into the problem. This enables the use of vectorized solvers like Block Krylov methods that improve hardware utilization for matrix-based simulations on modern hardware architectures.
Reformulating the all-at-once system we will obtain a matrix equation for multiple consecutive time steps that can be solved using vectorized solvers. The approach is applicable to a wide range of linear and nonlinear problems. We demonstrate its potential by presenting some numerical results for a realistic porous media application based on Richards' equation.

**Adaptive matrix-free simulations of fluid-filled phase-field fractures with fixed-stress coupling and fracture-width computation**

Kolditz, Leon (1); Wick, Thomas (1); Lee, Sanghyun (2); Kosin, Viktor (1,3)
*1: Leibniz Universität Hannover, Germany*
*2: Florida State University, USA*
*3: École normale supérieure Paris-Saclay, France*

17:30

Fluid-filled phase-field fracture simulations require robust, scalable solvers that can handle strongly nonlinear, non-smooth mechanics and tightly coupled flow on locally refined meshes. In this work, we develop an adaptive finite element framework for quasi-static, fluid-filled phase-field fractures that combines semi-smooth Newton methods, fixed-stress iterative coupling, and matrix-free geometric multigrid preconditioning. The geomechanics subproblem, with displacement and phase field as primary variables, is solved by a semi-smooth combined Newton method based on a primal–dual active set formulation. The resulting linear systems are treated with generalized minimal residuals and matrix-free geometric multigrid preconditioners on locally refined meshes, with a careful treatment of hanging nodes in the multigrid hierarchy and in the active set updates. The pressure equation is coupled to the mechanics via a fixed-stress iterative scheme, and each flow subproblem is likewise preconditioned by matrix-free geometric multigrid on the same adaptive meshes.

In addition, we introduce an enhanced fracture-width computation, inspired by and extending existing phase-field aperture formulas, to obtain more accurate and mesh-robust width fields consistent with the regularized fracture profile. The overall computational framework is demonstrated on a set of two- and three-dimensional benchmark problems, highlighting its robustness, efficiency, and accuracy for simulating fluid-filled phase-field fractures with local mesh refinement.

**Least-Squares based Error Estimates for Nonlinear Problems: On a Unified Framework and its Application to Poro-Elasticity**

Brodbeck, Maximilian (1); Schneider, Henrik (2); Bertrand, Fleurianne (3); Ricken, Tim (1)
*1: University of Stuttgart, Germany*
*2: University of Duisburg-Essen, Germany*
*3: University of Technology Chemnitz, Germany*

17:50

Porous materials exhibit complex interactions between the deformation of a solid skeleton and the flow of an interstitial fluid. Thermodynamically consistent models, such as the Theory of Porous Media (TPM), lead to coupled, nonlinear partial differential equations. When solved numerically, accuracy deteriorates in problems featuring re-entrant corners, internal- or boundary layers and shock-like fronts [1].

A-posteriori error estimates offer a systematic way to retain accuracy through localised mesh refinement but require information about the error distribution. Therefore, the first part of this talk introduces a unified framework establishing conditions under which a nonlinear Least-Squares functional can serve as error estimator for a class of nonlinear problems with specific structure [2].

This framework is then applied to the TPM, where linear approximations can cause severe violations of underlying conservation principles [3]. The application of a Least-Squares-based discretisation is demonstrated, while a brief outlook on how the proposed error estimator can be integrated into standard displacement–pressure-based code frameworks concludes the talk.

**References:**

[1] Verfürth, R. (1994). A posteriori error estimation and adaptive mesh-refinement techniques. J. Comput. Appl. Math., 50, p. 67-83.

[2] Bertrand, F. et al. (2025). Least-Squares Finite Element Methods for nonlinear problems: A unified framework, arXiv

[3] Brodbeck, M. et al. (2025). Phase transition in porous materials: effects of material parameters and deformation regime on mass conservativity. Comput. Mech., 75, p. 1191–1212.

**Toward Physics-Informed Operator-in-the-Loop Hybrid Solvers for Poroelasticity**

Mandl, Luis (1,2,3); Nayak, Dibyajyoti (3); Goswami, Somdatta (3); Ricken, Tim (1) 18:10

*1: Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Stuttgart, Germany*
*2: Experimental Hepatobiliary Surgery Group, Department of Hepatobiliary Surgery and Visceral Transplantation, University of Leipzig Medical Center, Leipzig, Germany*
*3: Department of Civil and Systems Engineering, Johns Hopkins University, Baltimore, Maryland, U.S.A*

Machine learning surrogates enable near real-time inference by moving expensive computation offline. Yet, beyond unit-domain benchmarks, these surrogates can lose accuracy and stability over long time horizons. A pragmatic scientific machine learning response is to hybridize learning and numerics. Deep operator networks (DeepONet) offer a general neural-operator template for learning mappings between function spaces, and HINTS [1] alternates DeepONet updates with classical relaxation steps until the residual is small.

Building on that idea, we pursue a physics-informed operator-in-the-loop framework that replaces repeated temporal or iterative updates with a learned operator. Each proposal is checked by a residual criterion: accept if small, otherwise switch to a classical solver update. The driving application is a poroelastic, multiphase, multiscale liver model within the theory of porous media (cf. [2]), but the formulation is solver-agnostic for update-driven schemes.

To reduce reliance on labeled simulations or experiments, we train with physics-informed operator learning by enforcing partial differential equation, boundary, and initial constraints. This also makes separability practical: independently sampled collocation points avoid the need for aligned full-field snapshots, which is often restrictive in purely data-driven training. Concretely, we build on separable physics-informed DeepONet [3], which factorizes coordinates into independent trunk subnetworks and uses forward-mode automatic differentiation to obtain linear scaling with dimension. On a 2D Biot consolidation benchmark, this yields a 98% speed-up.

For long-time extrapolation, we draw on physics-informed time-integrated operator learning [4]: the network learns the temporal tangent from the current state and advances it with standard integrators, while residual monitoring provides a lightweight drift indicator. This improves benchmark performance by up to 87% versus rollout baselines and shows a near-linear correlation between residual error and tangent error. The same residual-gated logic is consistent with data-driven hybrid switching ideas such as ANCHOR [5], which uses residual-based monitoring to trigger online switching between a pre-trained neural operator and a high-fidelity solver.

Taken together, these components support an operator-first workflow with residual-gated safeguards: fast when the operator is reliable, and corrected by classical updates when it is not.

[1] - Zhang et al., Nat Mach Intell 6, 2024, DOI: 10.1038/s42256-024-00910-x
[2] - Tautenhahn et al., GAMM-Mitteilungen 47, 2025, DOI: 10.1002/gamm.202370003
[3] - Mandl et al., CMAME 434, 2025, DOI: 10.1016/j.cma.2024.117586
[4] - Mandl et al., 2025, arXiv:2508.05190
[5] - Roy et al., 2025, arXiv:2512.19643

## YRM3: Quantum Computing in Applied Mathematics and Mechanics

Organizer(s): Kaseb, Zeynab *(Delft University of Technology)*
Berberich, Julian *(University of Stuttgart)*

## YRM3: Quantum Computing in Applied Mathematics and Mechanics

Date: March 16, 2026 16:30–18:30
Room: KII, M17.02
Chair(s): Berberich, Julian
Kaseb, Zeynab

### An introduction to quantum algorithms and their robustness

Berberich, Julian 16:30
*University of Stuttgart, Germany*

Quantum computing is a fascinating interdisciplinary research field that promises to revolutionize computing by efficiently solving previously intractable problems. Recent years have seen tremendous progress in the field but realizing computational advantages of quantum computers in practice remains a widely open problem due to numerous fundamental challenges. Interestingly, many of these challenges are connected to concepts and tools that are central in engineering and mathematics. This talk will provide a tutorial introduction to quantum computing from a mathematical perspective. I will introduce the framework of quantum algorithms ranging from basic elements including quantum bits and quantum gates to more advanced concepts. Moreover, I will discuss challenges in the field, especially related to the robustness of quantum algorithms, and outline how the GAMM community can help to overcome them.

### Nonlinear Quantum Computation by Amplified Encodings

Deiml, Matthias; Peterseim, Daniel 17:10
*Universtiy of Augsburg, Germany*

This talk presents a framework for nonlinear quantum computation suitable for solving high-dimensional problems, such as discretized nonlinear partial differential equations. The approach is based on the classical Newton's method, which through its fast convergence allows to preserve typical quantum advantages. In particular the memory and runtime required for the quantum method scales only logarithmically with the number of degrees of freedom.

### Solving complex systems of equations with quantum annealing

Kaseb, Zeynab; Moller, Matthias 17:30
*Delft University of Technology, Netherlands, The*

As power system problems grow in size and complexity, classical numerical solvers face increasing computational challenges. At the same time, emerging fault-tolerant quantum hardware offers the promise of improved scalability and computational speed-up. In this work, we introduce a combinatorial optimization framework that reformulates continuous power system problems into a form suitable for quantum and digital annealers. The framework supports both real and complex variables and can represent linear and nonlinear equations. To illustrate its capabilities, we present two case studies: (i) parameter identification, where the admittance matrix is estimated from voltage and current measurements, and (ii) power flow analysis, solving for active and reactive power balance. Our results demonstrate that the framework can effectively and efficiently address both tasks, highlighting its potential as a versatile tool for future power system applications.

**Performance enhancing of hybrid quantum-classical Benders' algorithm for MILP optimization**

López-Baños, Sergio (1,2); Lobe, Elisabeth (3); Lünsdorf, Ontje (1); Raventós, Oriol (1) 17:50

*1: German Aerospace Center (DLR), Institute of Networked Energy Systems, Carl-von-Ossietzky-Str. 15, 26129 Oldenburg, Germany*

*2: Hamburg University of Technology, Institute for Quantum Inspired and Quantum Optimization, Blohmstraße 15, 21079 Hamburg, Germany*

*3: German Aerospace Center (DLR), Institute of Software Technology, Lilienthalplatz 7, 38108 Brunswick, Germany*

Mixed-integer linear programming problems are extensively used in industry for a wide range of optimization tasks. However, as they get larger, they present computational challenges for classical solvers within practical time limits. Quantum annealers can, in principle, accelerate the solution of problems formulated as quadratic unconstrained binary optimization instances, but their limited scale currently prevents achieving practical speedups. Quantum-classical algorithms have been proposed to take advantage of both paradigms and to allow current quantum computers to be used in larger problems. In this work, a hardware-agnostic Benders' decomposition algorithm and a series of enhancements with the goal of taking the most advantage of quantum computing is presented. The decomposition consists of a master problem with integer variables, which is reformulated as a quadratic unconstrained binary optimization problem and solved with a quantum annealer, and a linear subproblem solved by a classical computer. The enhancements consist, among others, of different embedding processes that substantially reduce the pre-processing time of the embedding computation without compromising solution quality, a conservative handling of cut constraints, and a stopping criterion that accounts for the limited size of current quantum computers and their heuristic nature. The proposed algorithm is benchmarked against classical approaches using a D-Wave quantum annealer for a scalable family of transmission network expansion planning problems.

**Symbolic & parametric quantum circuit evaluation for tailored circuit optimization**

Ahrend, Oliver; Hegde, Sathyamurthy; Kowalski, Julia 18:10

*Chair of Methods for Model-based Development in Computational Engineering (MBD), RWTH Aachen University, Germany*

Quantum circuits are inherently parametric. This can be noted explicitly, e.g. by variational quantum algorithms (VQAs), for which classical optimizers are used to determine optimal sets of gate-parameters iterating between circuit evaluation and parameter update, or implicitly, e.g. in the quantum singular value transform (QSVT), for which "optimal" gate-parameters are determined a-priori only once. In general, the parameter space might fundamentally differ from the respective classical algorithms. For example, quantum neural networks (QNNs) form a highly oscillatory parameter space due to trigonometric functions in the gates, while classical NNs typically make use of monotonic activation functions.
Additionally, even in the advent of quantum error correction (QEC), fundamental challenges remain, and the optimal set of parameters depends strongly on hardware-characteristics, for instance, decoherence and limited precision controls. Experimental demonstrations of QEC for small scale circuits have been published, which seem scalable with larger numbers of qubits, but as circuits grow in depth, proof-of-concepts are missing [1].

Overall, reliable optimization of quantum circuits requires a case-by-case investigation. Established numerical simulation frameworks are well suited for evaluating the gate-driven linear mapping between quantum states $|\psi\rangle \leftarrow \mathrm{G}|0\rangle$, but the problem at hand is based on highly non-linear relations between parameters and state amplitudes $|\psi(\Theta)\rangle \leftarrow \mathrm{G}(\Theta)|0\rangle$, for which suitable tools have not yet been presented. The first challenge such a tool faces is to formulate the non-linear dependence.

In an attempt to make circuit-agnostic quantum-physical models, that describe individual gates, accessible to analysis of high-level quantum circuit descriptions, we present a symbolic quantum circuit simulator. It provides a symbolic and parametrized representation of the state and its evolution during circuit evaluation. This representation can be used to compute gradients, evaluate sensitivities,

or plot cost/energy/error landscapes. Ultimately, this allows us to understand in more detail how an algorithm behaves w.r.t. any kind of parameter we are capable of representing symbolically.

By interfacing with the OpenQASM circuit representation, our simulator primarily facilitates the exchange of circuits with established numerical simulation frameworks, such as Qiskit, Pennylane, etc., while also functioning as a stand-alone tool.

We will demonstrate the feasibility of this approach on a selected use case of quantum neural network (QNN) training. This insight enables to understand why popular classical optimizers ADAM and COBYLA require extensive tweaking to provide decent QNNs in our case, and motivates the development of dedicated optimizers.

[1] Quantum error correction below the surface code threshold. Nature 638, 920–926 (2025). https://doi.org/10.1038/s41586-024-08449-y

## YRM4: Simulation & control of flexible multibody systems

Organizer(s): Capobianco, Giuseppe *(FAU Erlangen-Nürnberg)*
Kinon, Philipp L. *(Karlsruhe Institute of Technology (KIT))*

## YRM4: Simulation & control of flexible multibody systems

Date: March 16, 2026 16:30–18:30
Room: KI, M11.62
Chair(s): Kinon, Philipp L.
Capobianco, Giuseppe

### Efficient computational modeling of nonlinear beam networks

Le Clézio, Helen (1); Lestringant, Claire (2); Karapiperis, Konstantinos (3); Kochmann, Dennis M. (1) 16:30
*1: ETH Zurich, Switzerland*
*2: Sorbonne Université, Paris, France*
*3: Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland*

Beam-based architected materials can be subjected to large strains in a range of applications. Finding efficient and accurate models for these materials at finite strains is a challenging task as their microstructure consists of many individual slender beam members that exhibit nonlinear effects due to their geometry (large rotations) and behavior (e.g., hyperelastic materials). Classical 1D models ignore nonlinearities due to advanced constitutive laws and full 3D finite element analysis comes at a prohibitive computational cost. Therefore, there is a need for an efficient modeling approach capable of accurately capturing the physics of these large, complex systems. Following a formal asymptotic dimension reduction approach, we decompose the problem into an efficient macroscale simulation of the beam's centerline and a finite elasticity problem on the cross-section (microscale) at each point along the beam. From the solution on the microscale, an effective energy is passed to the macroscale simulation, where it serves as the material model.
However, this two-scale approach comes at a high computational cost as it involves solving the microscale problem on the cross-section in a finite strain setting using finite element analysis. To leverage the efficiency of the macroscale beam simulation, we therefore introduce two approaches to increase the efficiency of the microscale simulations: The effective energy can be computed a priori for a catalog of macroscopic strain combinations for a given cross-sectional geometry and constitutive law(s) of the base material(s) within the cross-section. By introducing a third-order 4D interpolation, an approximate albeit smooth and differentiable energy landscape is obtained, which then serves as the material model for the macroscale simulation. Alternatively, the microscale simulations are substituted with a Sobolev-trained thermodynamics-informed neural network, which serves as a surrogate model for the costly microscale simulations. We demonstrate the effectiveness of our models in a suite of examples, ranging from cantilever beams to 3D beam networks.

References:
H. Le Clézio, C. Lestringant and D.M. Kochmann. A numerical two-scale approach for nonlinear hyperelastic beams and beam networks, IJSS (2023).
H. Le Clézio, K. Karapiperis and D.M. Kochmann. Nonlinear two-scale beam simulations accelerated by thermodynamics-informed neural networks, EML (2024).

### Simulation and parameterization of nonlinear elastic bending behavior in slender cables

Zhao, Tian (1,2); Schneider-Jung, Fabio (1); Linn, Joachim (1); Müller, Ralf (2) 16:50
*1: Mathematics for the Digital Factory, Fraunhofer Institute for Industrial Mathematics ITWM, Germany*
*2: Department of Civil and Environmental Engineering, Technical University of Darmstadt*

This work presents a computational framework for simulating and characterizing the nonlinear elastic bending behavior of slender structures, with a focus on cables.

Linn et al. [1] provide a robust framework for cable simulation based on Cosserat rod theory, where static equilibrium is obtained by minimizing the potential energy. However, this framework is restricted to linear elasticity. For real cable assemblies, especially those with complex structures, nonlinear elastic bending behavior is observed [2].
To address this, we introduce the Method of Iterative Linear Elastic Sub-problems (MILES). MILES solves the nonlinear elastic problem by iteratively minimizing the potential energy of a linear elastic sub-problem with constant algorithmic bending stiffness values, which are updated according to the current cable configuration and a prescribed curvature-dependent bending stiffness characteristic. The iteration proceeds until convergence is achieved.

In addition, we propose an experimental identification method that derives the curvature-dependent bending stiffness characteristic directly from measured reaction forces and the deformed centerline of the cable. The identified bending stiffness characteristic is used in MILES, and the corresponding simulations exhibit good agreement with bending tests performed on real cable specimens.
[1] J. Linn, T. Hermansson, F. Andersson, and F. Schneider. Kinetic aspects of discrete Cosserat rods based on the difference geometry of framed curves. In: M. Valasek, et al. (eds) Proceedings of the ECCOMAS Thematic Conference on Multibody Dynamics, pages 163-176. Prague, Czech Republic, 2017.

[2] V. Dörlich, J. Linn, S. Diebels. Flexible beam-like structures - experimental investigation and modeling of cables. In: Altenbach, H., Jablonski, F., Müller, W., Naumenko, K., Schneider, P. (eds) Advances in Mechanics of Materials and Structural Analysis. Advanced Structured Materials, Springer, Cham, 80:27-46, 2018.

**Robust and fast simulation of nonlinear rods in flexible multibody systems**

Herrmann, Marco (1); Breuling, Jonas (2); Cortes Garcia, Idoia (1); Eugster, Simon R. (1)

*1: Eindhoven University of Technology, the Netherlands*
*2: University of Stuttgart, Germany*

17:10

The computational complexity of multibody systems increases significantly when flexible components are included. This is not only due to the larger number of degrees of freedom, but also to their nonlinear coupling. In the case of highly flexible slender structures, here Cosserat rods, these additional degrees of freedom typically parametrize positions and cross-section orientations. We employ Lagrange interpolation of nodal positions and quaternions, combined with a Petrov–Galerkin projection, which ensures an objective and path-independent finite element discretization within a total Lagrangian framework. Moreover, independently interpolating the resultant contact forces and moments within the variational Hellinger–Reissner principle yields a mixed formulation that is locking-free and substantially more robust.
Compared to standard displacement-based approaches, the proposed formulation exhibits improved numerical convergence and robustness for both the nonlinear equations of motion and the nonlinear static equilibrium. The mixed formulation requires fewer Newton iterations and admits larger load increments in static simulations. We also identify a conceptual analogy to the so-called "lifted Newton method", where auxiliary variables are introduced to enhance the convergence behaviour of the Newton–Raphson root finding.
Beyond these numerical advantages, our approach naturally incorporates constrained rod theories, such as shear-rigid or inextensible models, in which the additional degrees of freedom act as Lagrange multipliers enforcing the respective deformation constraints.

**Adaptive implicit Runge-Kutta methods for stabilized index-one differential-algebraic equations in flexible multibody systems**

Breuling, Jonas

*University of Stuttgart, Germany*

17:30

Accurate and efficient time integration of stiff differential–algebraic equations (DAEs) is crucial for modern flexible multibody system (FMBS) simulations. The governing equations of motion typically form index-three DAEs, which are inherently ill-posed and pose severe challenges for standard time

integration schemes such as backward differentiation formulas (BDF). While stiffly accurate implicit Runge–Kutta (IRK) methods offer an attractive alternative, they often suffer from order reduction and require substantial modifications to existing implementations.

To overcome these difficulties, Anantharaman and Hiller (1991) proposed a stabilized index-one formulation that reformulates the FMBS equations into well-posed index-one DAEs. This transformation enables the direct use of existing implicit integration methods, such as BDF and IRK, without invasive changes. Building on this framework, this talk focuses on adaptive implicit Runge–Kutta methods, with particular emphasis on the three-stage, fifth-order Radau IIA scheme implemented in Hairer and Wanner's RADAU5.f code. The method is generalized to an arbitrary number of odd stages and applied to fully implicit DAEs of the form $F(t, y(t), y'(t)) = 0$.

The presentation concludes with numerical experiments on benchmark problems with known analytical solutions, demonstrating the accuracy, robustness, and efficiency of the proposed adaptive IRK approach for stabilized index-one FMBS formulations.

**Multibody Models Generated From Images: From Sketches to Simulation**

Manzl, Peter; Pieber, Michael; Möltner, Tobias; Gerstmayr, Johannes 17:50
*University of Innsbruck, Austria*

With the rise of Large Language Models (LLMs), natural language processing has found new applications not only in general-purpose conversation and code generation, but also in the creation of multibody (simulation) models. The latter requires both language processing capabilities and engineering knowledge, for example, how gravity, inertia, or joints function. A multibody system can be described textually, as in our previous work, or graphically. Although modern LLMs can readily produce executable code, validating the resulting models is substantially more difficult. For users, graphical descriptions are often more practical, particularly for specifying spatial relationships in mechanical systems.

We propose a framework using a multi-step LLM pipeline to generate and validate multibody models from graphical descriptions in the form of sketches. A vision language model (VLM) parses the image, identifying components and connections. While the VLM can also produce code directly, initial tests showed that assigning vision and coding to two dedicated models improves performance; thus, the vision model is instructed to create an intermediate representation (IR), which is a structured, unambiguous representation of the physically relevant information. Based on the IR, a second LLM specialized in coding is used to generate the corresponding multibody models. The generation of simulation models is split into two steps: first, the retrieval of context, and second, the creation of the corresponding code. In the retrieval step, the model determines which simulation elements are needed and chooses from a list, e.g., revolute joint, torque, gravity, or ANCF beam. For each selected element, a descriptive context is compiled, including short documentation, an example function call with arguments that explain how to use the simulation element. After code generation, executability and physical correctness of the simulation model are evaluated by executing it and comparing it with the ground-truth model. By automatically generating sketches from the generated simulation models, the vision model can verify, e.g., the initial configuration, even in the absence of ground truth.

Besides hand-drawn sketches, additional sketches are rendered automatically from simulation models to enable evaluation of thousands of images generated from parametrized ground-truth models. Open-weight models are run on local GPUs to enable reproduction of the results and local data handling. The multi-LLM pipeline shows promising initial results on a variety of simple simulation problems with 100% executability. Future work could include video-based verification, allowing the assessment of time-dependent behavior and dynamic consistency.

**Using a Modular Successive Approach For Model Inversion of Multibody Systems with Unstable Internal Dynamics**

Hochdahl, René; Seifried, Robert 18:10
*Hamburg University of Technology, Germany*

Adaptive trajectory tracking of rigid and flexible multibody systems requires advanced control strategies that are often model-based. The combination of a model-based feedforward controller with a robust model-free feedback controller is a promising approach. For this, the inverse model can be derived by establishing servo-constraints that force the control output to follow a predefined trajectory, resulting in a differential-algebraic equation. However, the computational effort for such a model inversion increases significantly for larger and more complex multibody systems. This is especially evident for systems with higher relative degree and systems exhibiting unstable internal dynamics. In the latter case, inverse models cannot be integrated forward in time but instead require solving a boundary value problem (BVP).

In order to reduce the computational effort, this contribution attempts to exploit the topology of such systems. Consider a multibody system with unstable internal dynamics and a topology that allows it to be modelled as two connected single-input single-output subsystems. Moreover, one subsystem contains the control input while the other contains the control output of the combined system. To reduce the overall computational effort, it is proposed in this contribution to reduce the size of the BVP by inverting these subsystems successively.

## YRM5: Interfaces between Optimal Control and Machine Learning

Organizer(s): Vásquez-Varas, Donato *(University of Chile)*
Walter, Daniel *(Humboldt-Universitat zu Berlin)*

## YRM5: Interfaces between Optimal Control and Machine Learning

Date: March 16, 2026 16:30–18:30
Room: KII, M17.01

### Localized actuators for parabolic systems: stabilizability and learning of optimal setups

Walter, Daniel 16:30
*Johannes -Kepler Universität Linz*

The present talk is split in two parts: First, we show that a broad class of nonautonomous, linear parabolic systems is stabilizable by a finite number of localized actuators each acting on a single point of the spatial domain. Stabilizing feedback controllers, both, explicit as well as optimal ones, are constructed. The second part of the talk revolves around improving the actuator setup by optimizing the number of employed actuators as well as their positions. We model this task as a nonsmooth minimization problem including a Riccati equation as a constraint. After proving its well-posedness and deriving first-order optimality conditions, a greedy minimization algorithm is employed for its solution. The talk is concluded by extensive numerical experiments confirming the presented theoretical results

### Optimization-Free Diffusion Model - A Perturbation Theory Approach

Khoo, Yuehaw (1); Peng, Yifan (1); Oster, Mathias (2) 16:50
*1: CCAM, University of Chicago, Chicago, USA*
*2: RWTH Aachen, Germany*

Diffusion models have emerged as a powerful framework in generative modeling, typically relying on optimizing neural networks to estimate the score function via forward SDE simulations. In this work, we propose an alternative method that is both optimization-free and forward SDE-free. By expanding the score function in a sparse set of eigenbasis of the backward Kolmogorov operator associated with the diffusion process, we reformulate score estimation as the solution to a linear system, avoiding iterative optimization and time-dependent sample generation. We analyze the approximation error using perturbation theory and demonstrate the effectiveness of our method on high-dimensional Boltzmann distributions and real-world datasets.

### Parametrization of semi-concave functions applied to Optimal Feedback synthesis

Vásquez-Varas, Donato (1,4); Kunisch, Karl (2,3) 17:10
*1: University of Chile, Chile*
*2: Johann Radon Institute for Computational and Applied Mathematics, Austria*
*3: University of Graz, Austria*
*4: Center for Mathematical Modelling, Chile*

The synthesis of feedback laws for optimal control problems is a challenging topic with a wide range of applications in engineering and the sciences. Classical methods for creating optimal feedback laws are based on dynamic programming. However, they suffer from the so-called *curse of dimensionality*,namely, the exponential growth of computational cost with the dimension of the problem.

To address this difficulty, in this talk we present a machine learning–based approach for approximating semiconcave functions and its application to control problems. The key ingredient of this methodology is a parametrization capable of preserving the semiconcavity of the function. In particular, this makes it possible to approximate the value function of a control problem while simultaneously obtaining performance bounds for the associated feedback. Finally, we present numerical experiments that highlight the advantages of this approach.

**Probabilistic Surrogate Models using Flow Matching**

Harder, Hans 17:30
*Paderborn University, Germany*

Surrogate models for dynamical systems play an important role in many applications. They substitute expensive simulations and can typically deal with imperfect real-world data or lack of information. Insofar, they are often crucial components in control-based applications. My presentation will focus on fast probabilistic surrogate models based on conditional flow matching, suitable for forecasting partially-observed systems. I want to demonstrate that these models are capable of generating high-quality samples in a timely manner, opening the door to interesting new applications.

**Separable approximations of optimal value functions and their representation by neural networks**

Sperl, Mario (1); Saluzzi, Luca (2); Kalise, Dante (3); Grüne, Lars (1) 17:50
*1: University of Bayreuth, Germany*
*2: University of Ferrara, Italy*
*3: Imperial College London, United Kingdom*

In this talk, we study the representation of high-dimensional optimal value functions using neural networks. We first show that neural networks can approximate separable functions with a number of neurons that grows only polynomially in the state-space dimension, thereby mitigating the curse of dimensionality for this class of functions. Building on this observation, we demonstrate how an intrinsic decaying sensitivity property of optimal control problems can be exploited to obtain separable approximations of optimal value functions. In particular, we show that decaying sensitivity allows the value function to be approximated as a sum of localized contributions, reflecting the diminishing influence of distant state variables. We discuss how such a property arises under uniform stabilizability and detectability assumptions in the linear setting and present first results toward extending this framework to nonlinear control systems. The theoretical findings are supported by numerical experiments in which neural networks are used to approximate high-dimensional optimal value functions.

**Tensor-Train-Based Semi-Lagrangian Schemes for High-Dimensional Mean Field Games**

Carlini, Elisabetta (1); Saluzzi, Luca (2) 18:10
*1: Sapienza, University of Rome*
*2: Università degli Studi di Ferrara, Italy*

Mean field games (MFGs) provide a powerful framework for modeling decision-making in large populations of interacting agents. However, solving high-dimensional MFG problems remains a significant computational challenge due to the curse of dimensionality. In this talk, we present a novel approach based on combining Semi-Lagrangian (SL) schemes with tensor-train (TT) decompositions to efficiently approximate solutions of high-dimensional MFGs. Semi-Lagrangian (SL) schemes allow us to derive a semi discrete in time approximations of the Hamilton-Jacobi-Bellman and Fokker-Planck-Kolmogorov equations, inherent in MFG models. By combining TT representations with SL discretizations, we achieve a scalable and memory-efficient numerical scheme that mitigates the exponential growth in computational complexity. We discuss theoretical properties of the method, numerical accuracy, and demonstrate its effectiveness through computational experiments on high-dimensional test cases.

# DFG Programs

## SPP 2256: Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials

Organizer(s): Schmidt, Bernd *(Universität Augsburg)*
Mosler, Jörn *(TU Dortmund University)*

## DFG-PP 2256: Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials

Date: March 17, 2026 14:00–16:00
Room: KII, M17.25

### Qualitative and quantitative analysis of a T3 structure in linearized elasticity

Tribuzio, Antonio 14:00
*University of Bonn, Germany*

In this talk, we study the rigidity properties of a differential inclusion in linearized elasticity. We will introduce and discuss a set K of three diagonal strains that are pairwise incompatible but with non-trivial (symmetrized) rank-1-convex hull. This is called a $T_3$ structure.
We first prove that K is rigid at the level of exact solutions, namely that Lipschitz maps whose gradient is locally in K must be affine. After this, we study the scaling behaviour of the corresponding singularly-perturbed elastic energy, giving quantitative information on the flexibility of K in the sense of approximate solutions.
This is based on a joint work with R. Indergand, D. Kochmann, A. Rüland, and C. Zillinger.

### Unconstrained approximation of problems with pointwise constraints

Bartels, Soeren 14:20
*University of Freiburg, Germany*

A well established approach to approximately solve variational problems with pointwise constraints is based on the discretization of corresponding gradient flows with a linearized treatment of the constraint in the time steps. This leads to unconditionally stable and convergent iterative schemes for detecting minimizers or low energy configurations. A drawback of the approach is that each time step requires the solution of a saddle-point system whose solution can be time-consuming. In order to only work with standard symmetric and positive system matrices we devise a scheme in which the correction is projected onto the tangent space related to the nonlinear constraints. We specify sufficient conditions for stability and convergence and provide bounds on the systematic error obtained in the constraint. Numerical experiments for liquid crystal applications and nonlinear bending problems show a significant improvement in computation time. This is joint work with Christian Palus (U Freiburg) and Lucas Bouck (Carnegie-Mellon U, USA).

**A Concept for the Coupling of Plasticity and Phase Transformation**

Gammer, Florian (2); Dinkelacker-Steinhoff, Sarah (1); Hackl, Klaus (1); Dolzmann, Georg (2) 14:40
*1: Ruhr Universität Bochum, Germany*
*2: Universität Regensburg, Germany*

Building on a previous work [1], we present a general model for elasto-plastic materials subject to linear kinematic hardening to describe the evolution of the microstructure associated with phase transformations. The model, based on the variational principles for inelastic materials, is formulated in strain space and incorporates the so-called dissipation distance for immediate development. However, the evolutionary phase development raises questions regarding its formation.
We establish a connection between this evolutionary approach, describing the volume fractions of the newly emerging phases and a microstructure continuously evolving in time, and a variational model, which we use to obtain the microstructure as a quasiconfexification. To perform this last step, we present certain techniques to determine the polyconvex and the respective rank-one convex envelope for our energy density. The initial results of this concept are explained using numerical simulations created with the programming language Julia including Finite Element Method (FEM) simulations.

**References**

[1] S. Dinkelacker-Steinhoff and K. Hackl, (2024), A general model of microstructure evolution including phase transformation in elasto-plastic materials, Proceedings in Applied Mathematics and Mechanics, 24, e202400024, https://doi.org/10.1002/pamm.202400024.

**Geometrically nonlinear Cosserat elasticity - How nonlinearities in the models PDEs influence regularity**

Gastel, Andreas; Hüsken, Vanessa 15:00
*University of Duisburg-Essen, Germany*

We want to give an overview of the progress achieved regarding regularity of Cosserat solids within the last six years.

Since the beginning of the 1900s, linear Cosserat elasticity is well known in the engineering community for modelling micro-polar elastic solids. But from a mathematician's perspective a geometrically nonlinear version of the model is interesting. Existence of solutions for the latter has been known for about 20 years, while regularity questions were investigated only very recently, after recognizing structures closely related to (p-) harmonic maps, a topic well known in the mathematics community.

Starting with the Cosserat bulk model, we present some different regularity results, for Cosserat energy minimizers as well as for critical points. It turns out that classical regularity theory for (p-) harmonic maps into manifolds is an essential tool in deriving those results. At the same time, the geometric nature of the model's nonlinearities in some cases allows
not only regular, but also quite singular solutions to exist. We demonstrate some geometric ideas behind those.

Finally, singular solutions do not exist, when we go away from the (3d-) Cosserat bulk
model towards a (2d-) Cosserat model for shells, both for initally flat or curved midsurfaces.

**Towards Robust Data-Driven Inelasticity for Spatially Two-Dimensional Problems**

Harnisch, Marius (1); Bartel, Thorsten (1); Schweizer, Ben (2); Menzel, Andreas (1,3) 15:20
*1: Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund, Germany*
*2: Department of Mathematics, TU Dortmund, Germany*
*3: Division of Solid Mechanics, Department of Construction Sciences, Lund University, Sweden*

By substituting traditional material models with datasets containing discrete pairs of stresses and strains, Kirchdoerfer and Ortiz [1] introduced the data-driven mechanics method. The solution of boundary value problems is derived directly from these data by minimizing a distance between the

discrete pairs, referred to as material states, and mechanical states, which satisfy equilibrium and kinematic compatibility.

While initially formulated for elastic materials, extending the method to path-dependent behavior of inelastic materials constitutes a crucial yet challenging step. In our previous work [2] we introduced a general framework for such evolutionary problems based on the concept introduced in [3]. It consists of a history surrogate, a quantity designed to store and compress the relevant information of the material's history, and an accompanying propagator that updates this history surrogate at the end of each time step. By enhancing both material and mechanical states with the history surrogate, our framework preserves the core characteristics of the original method, namely a global distance minimization between the enhanced states and a fixed data set not being modified during data-driven calculation.

As demonstrated in [2], for truss structures suitable choices of history surrogates and propagators can be constructed in an intuitive manner. However, for the complex stress and strain states of spatially two-dimensional problems, such intuitive approaches may become infeasible. Moreover, the challenges arising from the extensions go beyond the mere definition of a history surrogate, such as an initial state dependency exhibiting crucial effect on the accuracy of the data-driven solution. To address these challenges, we introduce a neural network-based propagator that autonomously learns an effective history surrogate and its evolution directly and purely from discrete stress-strain paths, in connection with an enhanced solution strategy.

In this contribution, we provide a thorough analysis of our enhanced framework's capabilities and current limitations. We extend the discussion to two-dimensional problems, analyze the additional challenges encountered in this setting, and present the corresponding enhancements and solution strategies developed to address them.

[1] T. Kirchdoerfer, M. Ortiz, Data-driven computational mechanics, Comput. Methods Appl. Mech. Engrg. 304 (2016), 81-101

[2] T. Bartel, M. Harnisch, B. Schweizer, A. Menzel, A data-driven approach for plasticity using history surrogates: Theory and application in the context of truss structures, Comput. Methods Appl. Mech. Engrg. 414 (2023), 116138

[3] K. Poelstra, T. Bartel, B. Schweizer, A data-driven framework for evolutionary problems in solid mechanics, J. Appl. Math. Mech. 103 (2023), e202100538

**Discrete-to-Continuum Limits of the Wave Equation on Time-Dependent Domains**

Correa, Santiago
*University of Augsburg, Germany*

15:40

In this talk, we study the wave equation with Dirichlet boundary conditions on time-dependent domains. We then prove that an atomistic model governed by Newtonian mechanics converges to the corresponding continuum solution, assuming that the domain grows over time and that the boundary moves with subsonic speed.

## SPP 2298: Theoretical Foundations of Deep

Organizer(s): Kutyniok, Gitta *(nan)*
Bülte, Christopher *(LMU München)*

## DFG-PP 2298: Theoretical Foundations of Deep

Date: March 17, 2026 14:00–16:00
Room: KI, M11.82
Chair(s): Bülte, Christopher

### Adversarial Training as a Primal-Dual Problem

Schmitt, Lucas 14:00
*Würzburg University, Germany*

An important topic in machine learning, particularly concerning security, is the robustness of models against adversarial attacks. This issue can be addressed through adversarial training, although this approach typically incurs high computational costs. In this work, we establish a characterization of the subdifferential of a nonlocal total variation functional, which is one-homogeneous and arises in a convex relaxation of the adversarial training problem for binary classification. To this end, we derive a dual representation of the nonlocal total variation involving a nonlocal divergence and gradient, and we ensure its consistency with their local counterparts. Based on this dual formulation, we develop a primal-dual algorithm for the relaxed adversarial training problem, providing an efficient algorithmic approach to solving the original problem.

### Anisotropic self-attention dynamics emerging from transformers with layer normalization

Burger, Martin (1,2); Kabri, Samira (1); Korolev, Yury (3); Roith, Tim (1); Weigand, Lukas (1) 14:20
*1: Deutsches Elektronen-Synchrotron DESY, Germany*
*2: University of Hamburg, Germany*
*3: University of Bath, United Kingdom*

Anisotropic self-attention dynamics emerging from transformers with layer normalization

Transformers and the associated (self-)attention layers, have proven to be successful machine learning architectures for a wide range of applications, including language processing with large language models. This practical success calls for a detailed mathematical understanding of such architectures. Recently, studying transformers from the perspective of interacting particle systems as proposed by Sander et al. (2022) has gained strong interest. The work by Geshkovski et al. (2024) connects the mean-field dynamics induced by self-attention layers equipped with layer-normalization to a time-continuous evolution of probability measures on a high dimensional sphere. In particular, it analyzes the long-time clustering behavior under isotropic interaction, which corresponds to a fixed choice of the so-called key, query and value parameters. In this talk, we relax these assumptions on the parameters towards a more practical setting such that the interaction between particles becomes anisotropic. We show how anisotropic interaction influences the stationary states of the dynamics on the sphere and discuss practical interpretations of the resulting long-time behavior. In an outlook, we point out possible implications for meta-stable states, multi-head attention and noisy transformers.

### Towards optimal control of ensembles of discrete-time dynamical systems

Fiedler, Christian 14:40
*Technical University of Munich (TUM) and Munich Center for Machine Learning (MCML), Germany*

In a variety of applications the problem of controlling an ensemble of non-interacting dynamical systems arises, most notably in quantum control, and most research efforts have been direced towards ensembles of continuous-time dynamical systems. However, in some application scenarios ensembles of discrete-time dynamical systems are naturally appearing. In particular, the training of deep

neural networks in a mean-field setting can be reframed as an optimal control problem of an ensemble of discrete-time dynamical systems. In light of these considerations, we establish some foundations of optimal control of ensembles of discrete-time dynamical systems, including existence results for optimal controls, and $\Gamma$-convergence results for the approximation of such optimal control problems. This is joint work with Alessandro Scagliotti.

**Weakly Convex Ridge Regularization for Accelerated 3D Non-Cartesian Parallel MRI Reconstruction**

Wache, German Shâma (1); Chaithya, Giliyar Radhakrishna (2,3); Neumayer, Sebastian (1) 15:00

*1: Chemnitz University of Technology, Germany*
*2: Inria, Parietal, Université Paris-Saclay, France*
*3: CEA, NeuroSpin, France*

The weakly convex ridge regularizer (WCRR) has shown great promise for 2D inverse problems. Yet its performance in 3D parallel imaging settings, particularly under non-Cartesian undersampling, remains largely unexplored. To address this gap, we extend the WCRR to the 3D multi-coil non-Cartesian MRI reconstruction framework. Furthermore, to account for the diversity of orientations inherent to volumetric anatomical structures, we introduce a rotation-invariant formulation that enhances the representational capacity of the regularizer without increasing the model complexity. The resulting regularizer is trained on a multi-noise-level denoising task and integrated into a variational reconstruction framework solved using a first-order optimization algorithm. We evaluate the proposed method on whole-brain 3D MRI data acquired with variable-density GoLF-SPARKLING trajectories and GRAPPA acceleration. Experimental results suggest that our method outperforms four popular baseline methods and is on par with the Plug-and-Play method coupled to the state-of-the-art DRUNet denoiser, while being significantly faster.

**Sampling in high dimensions and optimal transport**

Friesecke, Gero 15:20

*Technical University of Munich, Germany*

A common task in generative AI and molecular science is accurate sampling in high dimensions. In AI the underlying distribution has to be learned from data, whereas in equilibrium molecular dynamics the distribution is, in theory, known 'explicitly' from physical laws. In practice, and somewhat counter-intuitively, it has recently proven fruitful to 'forget' the explicit distributions and instead treat molecular sampling problems from a generative AI perspective. A particular challenge with molecular distributions is that they are typically not supported on low-dimensional manifolds, and non-smooth. In my talk I will explain how methods from optimal transport aid both the learning of, and the sampling from, the underlying distributions.

**Bayesian Unlearning in Generalized Linear(ized) Models**

Mucsányi, Bálint 15:40

*University of Tübingen, Germany*

There is an increasing need for principled yet efficient tools to unlearn knowledge from models. However, the conditions under which unlearning is successful are not yet well understood theoretically. We study efficient machine unlearning in Bayesian linear and linearized models. Starting from generalized linear models, we derive an efficient, single-step posterior downdate that is exact for linear regression and approximate for logistic regression. For the latter, we provide certificates: a lower bound on performance decrease on the data subset we aim to forget, and principal-angle bounds that cap the worst-case accidental forgetting of the retained subset. We further propose a constrained variant of the Bayesian edit, which enforces the preservation of retained-set performance. We lift the method and its bounds to modern neural networks through linearized Laplace approximations. On CIFAR-10/100, ImageNet, and Food-101, with ResNet and ViT models, our single-step downdates with scalable covariance approximations offer favorable forgetting-retention trade-offs compared to exact tangent-space unlearning, and our geometry-based certificates track empirical spillover.

## SPP 2311: Robust Coupling of Continuum-Biomechanical in Silico Models to establish active biological System Models for later use in clinical Applications - Co-design of Modeling, Numerics and Usability

Organizer(s): Röhrle, Oliver *(Universität Stuttgart)*
Ricken, Tim *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering (ISD))*

## DFG-PP 2311: Robust Coupling of Continuum-Biomechanical in Silico Models to establish active biological System Models for later use in clinical applications - Co-design of modeling, numerics and usablity

Date: March 17, 2026 14:00–16:00
Room: KII, M17.12

### Simulation, Surrogate Modeling and Parameter Optimization for Skeletal Muscle Models

Klink, Marian (1); Lautenschlager, Robin (1); Homs-Pons, Carme (2); Villota-Narvaez, Yesid (3); Doreti, Lalith Kumar (3); Göddeke, Dominik (1); Röhrle, Oliver (3); Schulte, Miriam (2)
*1: Institute of Applied Analysis and Numerical Simulation, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*
*2: Institute of Parallel and Distributed Systems, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*
*3: Institute for Modelling and Simulation of Biomechanical Systems, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*

14:00

The agonist-antagonist myoneural interface (AMI) is a novel clinical technique in which residual skeletal muscle pairs, for example after limb amputation, are functionally reconnected to restore proprioceptive feedback and improve the patient's neural and mechanical control. In current applications, decisive patient-specific physiological parameters are determined heuristically, such as the prestretch of the involved muscle pair, which directly influences the patient's range of motion. To support AMI surgical planning, we present a complete computational framework to determine optimal physiological parameters in three steps: First, we present a high-fidelity computational model of the AMI two-muscle-one-tendon system, including subcellular muscle processes, neural feedback loops and large-scale mechanical behavior. While this model accurately represents the complex interactions of the involved physiological systems, its computational cost is too high to permit the multiple simulation runs needed for parameter optimization in practical applications. Thus, in the second step, we propose a surrogate-modeling framework to approximate the key quantities of interest of the high-fidelity simulation, such as muscle range of motion and force production. Precisely, we construct data-driven surrogates based on data generated using the high-fidelity model to obtain an accurate and efficient approximation. Third and finally, we utilize the constructed surrogate model to optimize the key quantities of interest with respect to the physiological parameters. In a series of numerical experiments, we visualize the dependencies between selected physiological parameters and muscle range of motion and force production. Furthermore, we compare the optimization using the surrogate to the optimization using the high-fidelity model and demonstrate that the surrogate-based approach can recover the optimal physiological parameters while reducing the computational effort by orders of magnitude. Consequently, this framework provides an accurate and efficient tool to support AMI surgical planning.

**Computational Modeling of Growth and Remodeling in Tissue-Engineered Biohybrid Cardiovascular Implants**

Sesa, Mahmoud (1); Holländer, Jasmin (1); Reese, Stefanie (1,2); Linka, Kevin (1) 14:30

*1: RWTH Aachen University, Germany*
*2: University of Siegen, Germany*

Fabricating clinically viable tissue-engineered cardiovascular implants remains a significant challenge due to the demanding physiological loading conditions they must withstand. A promising strategy involves the development of biohybrid implants, where biocompatible textile scaffolds act as reinforcement. While initial scaffold architecture is critical, the long-term mechanical performance of these implants is strongly influenced by the mechanobiological response during the maturation process.

In this work, we present a thermodynamically consistent computational framework designed to model the evolution of biological tissues during the maturation process [1]. The framework describes volumetric growth and fiber reorientation using a stress-driven homeostatic surface approach, while an energy-based approach is employed to model collagen densification [2]. This predictive model is applicable to general boundary value problems and has been extended to incorporate fiber-reinforced textile scaffolds.

We performed in silico experiments on various structural examples, including uniaxially and biaxially constrained tissue constructs, textile-reinforced pressurized shell constructs, and tissue-engineered vascular grafts (TEVGs). Results indicate that mechanobiological adaptation plays a dominant role in mechanical response of the tissue, often counteracting pre-defined scaffold anisotropy. Collagen density and orientation evolve to maintain homeostasis regardless of the initial textile architecture. Global sensitivity analysis reveals that by the end of the cultivation process, growth and remodeling terms eventually dominate the stress response over the initial mechanical properties of the scaffold. Furthermore, our model identifies principal stresses arising from tissue contractility during the cultivation process of TEVGs as a key factor influencing fiber alignment.

**Extension of liver biomechanics framework for whole-body applications**

Gerhäusser, Steffen (1); Mandl, Luis (1,2); Dahmen, Uta (3); Tautenhahn, Hans-Michael (2); Ricken, Tim (1); König, Matthias (1,4) 15:00

*1: Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Germany*
*2: University of Leipzig Medical Center*
*3: Jena University Hospital*
*4: Humboldt University Berlin*

Liver transplantation is the only curative treatment for end-stage liver disease, but changing demographics and Western lifestyles are leading to an increase in elderly, multi-morbid donors and recipients. When faced with a marginal graft, surgeons must weigh the risks: accept a suboptimal organ with potential postoperative complications or reject it, increasing the recipient's chances of dying on the waiting list. Simulation-based risk assessment via a digital liver twin has enormous potential to evaluate and, if necessary, optimise or cancel the planned transplantation process in everyday clinical practice, e.g. modelling patient-specific impairment of liver grafts [1]. During the transplant procedure, the organ changes bodies from donor to recipient, but may also be linked to a perfusion machine as a conservatory measure. An important research question is how the different milieus affect liver function during and after the procedure. To investigate this, the existing tissue-scale model is coupled with an external third scale model (e.g., representing body or perfusion machine) to incorporate the influence of the surrounding environment. This is of particular interest as it enables the use of physiologically more realistic boundary conditions and allows the simulation of reperfusion scenarios compared to the standalone tissue-cell boundary value problem. In this work, the framework for coupling tissue-scale and cellular-scale processes based on FEniCSx [2], libRoadRunner [3], and preCICE [4] will be extended by an additional ODE-based physiologically based pharmacokinetic (PBPK) model [5]. We look into the theory, implementation, validation and challenges behind this ODE-PDE-ODE approach during simulation scenarios with clinical relevance.

**References:**

[1] Tautenhahn H. et al., GAMM-Mitteilungen, DOI:10.1002/gamm.202370003

[2] Baratta I. A. et al (2023). Zenodo. doi: 10.5281/zenodo.10447666.

[3] Welsh C. et al., Bioinformatics (2023)39

[4] Chourdakis G. et al. Open Research (2022)2

[5] Elias M. [1] et al (2025)., Frontiers in Pharmacology (2025)8

**Reaction–Diffusion–Transport Equations for Meniscus Regeneration Coupled with Biot's Equation**

Hussein, Ahmad (1,2); Surulescu, Christina (2); Simeon, Bernd (2) 15:30

*1: Ulm University*

*2: RPTU Kaiserslautern-Landau*

Tears of the meniscus are among the most common injuries, particularly in athletes and elderly patients. They can lead to severe chronic knee pain, stiffness, and reduced mobility, which may ultimately result in total knee replacement. Partial or total meniscectomy often causes long-term complications such as osteoarthritis. Tissue engineering offers promising alternatives for generating suitable regenerative tissue for meniscus replacement. However, most regenerative approaches are clinically driven and focus primarily on practical application rather than on the underlying micro- and macroscopic cellular mechanisms and their interactions with the scaffold material.

Mathematical models and numerical simulations therefore provide a valuable tool for understanding and analyzing the fundamental control mechanisms in cell–scaffold interactions under varying environmental conditions, enabling targeted predictions of the most favorable parameter combinations. The corresponding mathematical model consists of a system of coupled nonlinear parabolic PDEs describing the advection and (de)differentiation of mesenchymal stem cells and chondrocytes, while accounting for the anisotropy of the fibrous scaffold.

To include the mechanical stimuli, we compute both the differentiation medium flow through the porous scaffold medium and the mechanical deformation using Biot's equation. In this talk, we will present and compare different combinations of finite element spaces for the approximation of Biot's equation using continuous and discontinuous Galerkin methods in order to obtain a stable numerical approach. We compare the convergence rates and computational cost of the different discretization strategies using the open-source solver FreeFEM++. We also discuss possible implications for the mathematical model and for the in vitro experiment.

## SPP 2353: Daring More Intelligence – Design Assistants in Mechanics and Dynamics

Organizer(s): Eberhard, Peter *(University of Stuttgart - ITM)*

### DFG-PP 2353: Daring More Intelligence – Design Assistants in Mechanics and Dynamics

Date: March 17, 2026 14:00–16:00
Room: KI, M11.71
Chair(s): Eberhard, Peter
Rosenfelder, Mario

### A soft pneumatic actuator design assistant – from task to design

Schindler, Leon; de Payrebrune, Kristin 14:00
*RPTU University Kaiserslautern-Landau, Germany*

While conventional robots are intended to execute specific tasks in a controlled environment without external influences, they may pose harm when interacting with humans or might be unsuitable for operation in harsh environments. Soft robots, a subfield of continuum robots, can be used in such cases, where external influences are not determined or a specific versatility is required. Due to their soft and flexible structure, they deform continuously and can be used in a collaborative setting with humans or when handling fragile objects without applying large forces.
To achieve a general movement, a soft pneumatic bending actuator can be used to actuate a slender soft robot. Applying a specific air pressure in one of the air chambers results in a bending deformation of the actuator. However, when a particular bending motion should be achieved under a given pressure, the question of the optimal design of the soft pneumatic actuator arises. We present an inverse design process, which helps practitioners to tailor soft pneumatic actuators for specific tasks. We show that this inverse design process can be performed using genetic algorithms as a gradient-free optimization method while additionally complying with manufacturability constraints. Further, we present methods to enhance this design optimization with inverse surrogate models trained on the generated data.

### Generative Design of Acoustic Metamaterials Using Neural Operators

Dogu, Mert; Schmid, Johannes D.; Mörwald, Markus; Marburg, Steffen 14:20
*Technical University of Munich, Germany*

Acoustic metamaterials have emerged as a class of engineered materials that can manipulate sound waves beyond the limits of conventional materials. They enable precise control, absorption, and redirection of acoustic energy, allowing for advanced noise reduction and sound control solutions. Translating these concepts into practical, large-scale applications remains challenging due to design complexity, fabrication constraints, and the need for broadband performance. Overcoming these challenges requires efficient methods to navigate complex design spaces and predict metamaterial performance without the need for extensive iterative simulations. Considering solutions for these problems, data-driven approaches, particularly those leveraging machine learning, represent a promising direction addressed in this contribution. In this work, we focus on developing a data-driven generative design assistant for acoustic metamaterials based on operator learning. Neural operators, which learn mappings between function spaces, are employed to establish a relationship between a desired transmission loss spectrum and the corresponding absorber design parameters. Once trained on training datasets, the neural operator directly predicts the relationship between the function spaces without the need for iterative optimization. Acting as a surrogate model, it enables near-real-time design exploration, data fusion between simulations and experiments, and interactive parameter tuning. The proposed workflow integrates high-fidelity numerical simulations using finite element modeling with machine-learning-based neural operators to accelerate the development of next-generation metamaterial structures. The methodology of neural operators is demonstrated using different neural operator architectures. In future work, within the scope of Deutsche Forschungsgemeinschaft Priority Program “Daring More Intelligence - Design Assistants in Mechanics

and Dynamics" (SPP 2353), the project aims to extend this framework by combining physical modeling, operator learning, and inverse approaches, thereby establishing a robust, data-driven design assistant system for noise-reduction technologies in eVTOL systems. This will support faster, more reliable, and socially acceptable urban air mobility solutions.

**Nonlinear Model Predictive Control for a Lambda Robot based on Data-Driven surrogate model**

Hajipour, Sanam; Zhai, Tianyu; Bestle, Dieter 14:40
*Brandenburg University of Technology Cottbus-Senftenberg, Germany*

This work presents a nonlinear model predictive control (NMPC) framework for a lambda-shaped parallel robot which incorporates data-driven surrogates to facilitate control design. An inverse surrogate model is used to provide an efficient initialization of the control inputs in NMPC. The presented controller enables anticipation of the system behavior, enforces constraints, and optimizes the control performance over a finite prediction horizon.

The inverse surrogate model is trained using an appropriately constructed data set [1]. The resulting initialization is, therefore, already close to the optimal solution, which significantly accelerates the optimization process in the NMPC framework. To estimate the states and outputs within NMPC, an advanced multiple-shooting approach is employed instead of single shooting. This method performs state and output estimation over the entire prediction horizon simultaneously, thereby improving numerical robustness and convergence behavior.

Simulation results demonstrate that the proposed method achieves high accuracy and robust performance in the presence of disturbances. Furthermore, comparative studies with LQR and SMC controllers are conducted. The results indicate that the proposed method significantly outperforms a LQR controller [2], while exhibiting performance characteristics that are comparable to those of a SMC controller [1], where each approach shows distinct advantages depending on the specific operating conditions.

[1] Hajipour, S., Zhai, T., Bestle, D., Data-driven Sliding Mode Control of a Parallel 2D-Robot. *The 8th International Conference on Intelligent Robotics and Control Engineering (IRCE)*, Kunming, China, pp. 75-80, 2025. **doi:** 10.1109/IRCE66030.2025.11203089

[2] Bestle, D. and Hajipour, S., Design of a Tracking Controller Based on Machine Learning. *International Journal of Mechanical System Dynamics*, Vol. 5, No. 2, pp. 201-211, 2025. **doi:** https://doi.org/10.1002/msd2.70006

**On the Design of Model Predictive Controllers for Nonholonomic Multibody Systems**

Rosenfelder, Mario (1); Ebel, Henrik (2); Eberhard, Peter (1) 15:00
*1: Institute of Engineering and Computational Mechanics - University of Stuttgart, Germany*
*2: Department of Mechanical Engineering - LUT University, Finland*

Controlling nonholonomic systems is inherently challenging. Conventional linearization techniques fail to yield controllable approximations, as direct linear combinations of the system's input vector fields do not span the full tangent space of the configuration manifold. Instead, nested Lie brackets of the direct control vector fields must be employed to generate motion in directions that are not directly actuated. This fundamental property of nonholonomic systems is often addressed on kinematic level, where tailored model predictive control schemes have recently been developed that account for the underlying sub-Riemannian geometry by using a tailored cost function. Multibody systems, however, are naturally described by dynamic models that incorporate inertia, gyroscopic forces, and external forces. Preliminary studies indicate that in this dynamic context, possibly due to the increased state-space dimension, it appears that relying on conventional Euclidean distances becomes even more problematic. Hence, it is crucial to work with suitable geometric measures that take into account the dynamic system's nonholonomic nature.

The present work aims to address this gap by discussing how recent model predictive controllers - tailored for nonholonomic kinematic systems - can be systematically extended to precisely control

the dynamics of the corresponding multibody systems. The objective is to develop an easy-to-apply design assistant for optimization-based controllers tailored for nonholonomic multibody systems, assisting practitioners without the need for deep theoretical knowledge of the underlying geometric concepts. Beyond models that are purely based on first principles, it is further investigated how data-driven modeling techniques can be integrated into the optimization-based control framework. For example, enhanced kinematic models can be identified from readily available position-level data, while relying on first-principles-based models for the dynamic aspects, as acquiring high-quality data on velocity or acceleration level is typically more sophisticated. This hybrid modeling strategy allows data-driven components to complement analytical multibody models, improving predictive accuracy within the optimization-based control scheme. The effectiveness of the proposed methodologies is demonstrated on an exemplary nonholonomic multibody system.

**Indirect vs. Direct Methods for Periodic Trajectory Optimization in Legged Robots: Toward Co-Design Applications**

Raff, Maximilian (1); Flaßkamp, Kathrin (2); Remy, C. David (1)
*1: University of Stuttgart, Germany*
*2: Saarland University, Germany*

15:20

There exist two principal approaches for identifying optimal trajectories of dynamic systems: the *direct* and the *indirect* method.
The *direct method*, which is most widely used in practice, parameterizes the control inputs and optimizes them directly over a predefined finite-dimensional input space. This discretization typically leads to a high-dimensional nonlinear program but offers conceptual simplicity and considerable implementation flexibility. A key drawback is that the accuracy of the obtained trajectory is limited by the chosen parameterization; potentially superior solutions lying outside this discretization may be missed.
The *indirect method* offers a different approach by implicitly defining the control inputs as functions of the system's states and additional costates.
When combined with shooting methods and variable step-size integrators, it typically yields more accurate solutions.
While the introduction of costates formalizes the necessary first-order conditions, it does not substantially increase the dimensionality of the optimization problem. However, the resulting Hamiltonian dynamics are inherently conservative, which poses significant challenges for numerical convergence.

In this work, we address this convergence issue by constructing families of optimal motions for periodically operating systems. Convergence in these parameterized problems is maintained by remaining within the region of attraction using numerical continuation, which locally traces and connects optimal periodic orbits parameterized by a single operating condition.
Our target application is the generation of families of periodic walking motions (gaits) for legged robotic systems.
By continuously tracing gaits that originate from stand-still, we systematically generate gait families over a range of operating points, such as average walking speed.

A key insight enabling this tracing procedure is that periodic motions with zero actuation, including stand-still equilibria, are globally optimal solutions for energy-based cost functions.
These *passive* gaits therefore serve as ideal seed trajectories for generating gait families via numerical continuation.
As a primary contribution, we show how the costates that are necessary in the indirect method can be recovered from such an equilibrium or (quasi-) passive gait to fully initiate the continuation process.

Using these insights, we compare the direct and indirect approaches on two representative legged systems: the compass-gait walker and a model of RABBIT, a 5-link planar walking robot. Finally, we discuss how systematic generation of gait families can support the co-design of legged robots, enabling joint optimization of hardware design and the resulting trajectory optimization problems.

**Shape Optimization of a Hydraulic Turbine Using Deep Reinforcement Learning**

Eyselein, Simon; Rentschler, Tobias; Tismer, Alexander; Riedelbauch, Stefan 15:40
*University Stuttgart, Germany*

The present study explores the potential of Deep Reinforcement Learning for the geometric optimization of a hydraulic turbine and compares its performance with that of an Evolutionary Algorithm.

Shape optimization in fluid mechanics often leads to high-dimensional and highly non-linear problems, requiring efficient methods to approximate global optima. Evolutionary algorithms have been widely established, but they require a large number of function evaluations. In the case of turbine design, each evaluation involves a resource-intensive Computational Fluid Dynamics simulation. The optimization approach based on Deep Reinforcement Learning is grounded in policy gradient methods, where the agent learns a policy to generate turbine geometries that maximize a reward derived from the simulation results. The algorithm is designed to iteratively improve the geometry by sampling new configurations based on learned policies, guided by feedback from the Computational Fluid Dynamics evaluation.

A detailed model of an axial turbine, covering various aspects of the turbine's design and functionality, is parameterized by thirty design parameters in a test case. The optimization targets two main objectives: increasing the efficiency of the turbine and minimizing the cavitation volume, which is essential for the performance and durability of the turbine. Additionally, there is a constraint associated with the design head which has to be fulfilled.

The study reveals a critical limitation: the Deep Reinforcement Learning-Method converges toward regions in the parameter space associated with high average rewards, yet these regions do not consistently contain the highest-performing turbine geometries. In contrast, the Evolutionary Algorithm generates designs with superior fitness values, indicating that Deep Reinforcement Learning-Method favors regions of the design space associated with robustness to variations in design parameters but does not consistently identify the highest-performing solutions.

## SPP 2410: Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness

Organizer(s): Keim, Jens *(University of Stuttgart)*
Rohde, Christian *(University of Stuttgart)*

## DFG-PP 2410: Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness

Date: March 17, 2026 14:00–16:00
Room: KII, M17.52
Chair(s): Rohde, Christian
Keim, Jens

### On the Least Action Admissibility Principle in the Context of the Compressible Euler Equations

Pellhammer, Valentin 14:00
*Universität Konstanz, Germany*

Over the past decade, convex integration has profoundly altered our view of weak solutions to the multi-dimensional barotropic compressible Euler equations by exposing non-uniqueness, even for solutions that satisfy classical entropy conditions. In particular, convex integration has enabled the construction of infinitely many admissible weak solutions for certain Riemann-type initial data, showing that genuinely multi-dimensional solutions can emerge from data that are originally one-dimensional. Researchers have studied different selection criteria to rule out seemingly non-physical solutions, including approaches based on maximal energy dissipation. One recent idea is the least-action admissibility principle, which seeks to select solutions that minimize an action functional rooted in variational mechanics. In this talk, we give an overview of different selection criteria and their effectiveness, showing that they rule out a solution that is often regarded as the physically natural one. This suggests that either our understanding of a single physically relevant weak solution needs to be reconsidered, or the principles themselves must be discarded as viable selection criteria.

### Energy-variational framework: existence of solutions and selection criteria

Sliwinski, Marcel; Eiter, Thomas; Lasarzik, Robert 14:30
*WIAS Berlin, Germany*

We present the energy-variational framework in the context of a broad class of evolutionary partial differential equations. Building on earlier work on general conservation laws and abstract evolution equations, we extend the approach to encompass a wider range of systems. In particular, we consider new examples from fluid dynamics, which illustrate the adaptability of the framework. In addition to existence we present selection criteria, allowing to choose solutions with additional properties. This is a joint work with Thomas Eiter and Robert Lasarzik.

### Compressible Euler equations with Transport Noise

Boadi, Richard; Breit, Dominic; Moyo, Thamsanqacastern 15:00
*University of Duisburg-Essen, Germany*

We study the isentropic compressible Euler equations in multi-dimensions with stochastic perturbation of transport type. On the one hand, this is motivated by the physical modelling in turbulence theory. On the other hand, it has been shown recently that this type of noise can have regularising effects. In this work, we prove the existence of dissipative measure-valued martingale solutions and the weak-strong uniqueness property.

**Non-linear stability of shock profiles in dissipative hyperbolic-hyperbolic systems**

Sroczinski, Matthias 15:30
*Universitaet Konstanz, Germany*

In this talk, we prove nonlinear stability for smooth small-amplitude shock profiles
of second-order dissipative hyperbolic-hyperbolic systems under the assumption of spectral stability. This class of systems notably includes the two types of causal viscous relativistic gas models introduced respectively by Freistühler-Temple and Bemfica-Disconzi-Noronha, and (the equivalent second-order form of) a class of first-order numerical relaxation systems generalizing the well-known Jin-Xin relaxation schemes.
As a significant technical innovation, we present a new paradifferential-type nonlinear damping estimate
allowing the treatment of systems far from the symmetric structure required for the standard "Kawashima-type" energy estimates that are typically used for that purpose.

# Contributed Sessions

## S01: Multi-body systems, mechatronics and robotics

Organizer(s): Eberhard, Peter *(University of Stuttgart - ITM)*
Ebel, Henrik *(LUT University)*

## S01.01: Multi-body systems, mechatronics and robotics

Date: March 18, 2026 16:30–18:30
Room: KII, M17.51
Chair(s): Ebel, Henrik
Eberhard, Peter

### AI-Driven Generation and Assessment of Flexible Multibody Systems

Gerstmayr, Johannes; Weyrer, Sebastian; Möltner, Tobias; Manzl, Peter; Pieber, Michael 16:30
*University of Innsbruck, Austria*

Recent advances in large language models (LLMs) are expanding the range of algorithmic tasks that can be solved, including those traditionally requiring substantial domain expertise. Their application in engineering contexts raises critical concerns, as outputs may appear plausible without guaranteed correctness. The novelties and objectives of this work concernthe reliable and automated generation of simulation models, in particular concerning flexible multibody systems, together with their systematic validation. We extend the approach of recent work where simulation codes have been created by LLMs from textual descriptions of mechanical models to incorporate flexible bodies of different shapes and mechanical properties. In a bidirectional approach, one direction focuses on simplifying API interfaces to improve the usability of existing Exudyn functions for LLMs while the other direction builds on an automated model generation pipeline to systematically generate multibody systems. The model generation pipeline is divided into three steps: first, the LLM creates FEM objects, including geometry, finite element mesh, modal reduction and interfaces for flexible bodies. Second, the LLM preselects required simulation elements like rigid bodies, connectors, forces, and actuators. Third, the pipeline generates the simulation code for the multibody system, using context that includes implementation information and brief documentation on the previously created FEM objects and the selected simulation elements. In doing so, the LLM must also account for the interfaces of the FEM objects. Furthermore, the framework is extended beyond textual descriptions to also accept sketches and drawings of mechanical models. For evaluating the generated simulation codes and benchmarking LLM performance, we define reference implementations as ground truth and harmonize solver settings to ensure comparability. The evaluation separates executability and physical correctness: executability requires that the code runs to completion, while physical correctness is satisfied when deviations from the ground truth remain below a threshold. Additionally, the inertia properties and eigenfrequencies of LLM-generated FEM objects are validated against the ground truth. Previous results showed that the framework can reliably generate simulation code for rigid multibody models with an executability of up to 99.4% and physical correctness of up to 91.7%. Preliminary results of the proposed framework for flexible bodies indicate that LLMs can construct simple 3D flexible body geometries and interfaces, being able to generate flexible multibody systems beyond academic prob-

lems. The present approach has the potential to bring LLM-based generation of flexible multibody systems closer to industrial requirements, and to enable LLMs to support engineers of the future.

**Integration of a non-linear material model for filled elastomers in multi-body simulations of highly dynamic systems**

Niemeyer, Mascha; Woschke, Elmar; Juhre, Daniel 17:10
*Otto von Guericke University Magdeburg, Institute of Materials, Technologies and Mechanics*

Damping elements made of elastomers are commonly used in dynamic systems such as vehicles or centrifuges. al simulation methods, particularly multi-body simulation (MBS), are employed to predict loads and kinematic quantities in these technical systems. This requires knowledge of mass, damping and stiffness properties. Therefore, accurately modeling elastomer components is essential for achieving high prediction accuracy. However, the complex and extremely non-linear material behavior of elastomers [1] demands material models capable of replicating these mechanical properties. In addition, one-dimensional models may not suffice for modeling damping elements un-der multi-axial loading [2,3].

To enhance the prediction accuracy of MBS by incorporating these nonlinearities, the first step is to establish an MBS model for the dynamic system, using a laboratory centrifuge as an example. This forms the basis for gradually increasing the modeling depth, starting from a simple rheological model with the objective of substituting it with a physically-motivated material model. Thus, the force element in MBS is extended to be coupled with finite element analysis (FEA).

**Literature**

[1] M. Rendek and A. Lion. *Strain induced transient effects of filler reinforced elastomers with respect to the Payne-Effect: experiments and constitutive modelling*. Z. Angew. Math. Mech., 90: 436-458, 2010.

[2] X. Feng, P. Xu, and Y. Zhang. *Filled rubber isolator's constitutive model and application to vehicle multi-body system simulation: A literature review*. SAE International Journal of Vehicle Dynamics, Stability, and NVH, 2(2):101–120, 2018.

[3] J. Kadlowec, D. Gerrard, and H. Pearlman. *Coupled axial–torsional behavior of cylindrical elastomer bushings*. Polymer Testing, 28(2):139–144, 2009.

**A Mixed Discrete Cosserat Rod Formulation**

Dai, Tianxiang (1); Herrmann, Marco (2); Breuling, Jonas (1); Leine, Remco I. (1); Eugster, Simon R. (2) 17:30
*1: University of Stuttgart, Germany*
*2: Eindhoven University of Technology, The Netherlands*

Numerous parametrizations and discretization strategies have been developed for Cosserat rod theory, each with its own strengths and limitations. However, implementing any specific discretization is often challenging and typically requires a solid background in finite element methods together with expertise in handling large rotations. In this work, we show that, given a background in multibody dynamics, or assuming an existing rigid-body simulation framework, a Cosserat rod can be easily integrated into it. We demonstrate that a discretized Cosserat rod admits a natural interpretation as a sequence of rigid bodies with force and moment interactions that encode bending, torsional, shear, and axial resistance. These interactions are given as force laws in compliance form that relate discrete strains, computed from the positions and orientations of the rigid bodies, to internal forces and moments. The compliance form naturally also includes shear-rigid and inextensible versions of the Cosserat rod theory. Importantly, we show that the entire discrete multibody representation rigorously emerges from a mixed Petrov–Galerkin finite element formulation, providing a clear variational foundation for the method.

Finally, we analyze the spatial convergence behavior of the proposed formulation and demonstrate its applicability to soft robotic systems, in which Cosserat rods are ofen used to model continuum manipulators and other soft structures.

**Structure-preserving discretization of Cosserat rod dynamics in a mixed DAE-framework**

Kinon, Philipp L. (1); Eugster, Simon R. (2); Betsch, Peter (1) 17:50

*1: Karlsruhe Institute of Technology (KIT)*
*2: Eindhoven University of Technology (TU/e)*

Although the Cosserat rod model is well established, mixed formulations and corresponding finite element methods for its dynamic behavior remain relatively scarce. Likewise, only few works have explored Cosserat rods within the port-Hamiltonian (PH) framework, despite the framework's natural suitability for modeling complex interconnected systems.

To this end, we present an energy-based modeling framework for the nonlinear dynamics of spatial Cosserat rods undergoing large deformations and rotations. The mixed formulation employs independent configuration, velocity, and stress variables, ensuring objectivity and eliminating locking effects. Finite rotations are handled using a director-based parametrization that avoids singularities and results in a constant mass matrix. This leads to an infinite-dimensional nonlinear PH system governed by partial differential–algebraic equations with a quadratic energy functional.

A time-differentiated compliance representation of the stress–displacement relations enables the straightforward inclusion of kinematic constraints, such as inextensibility or shear rigidity. Dissipative material behavior (via generalized Maxwell models) and nonstandard actuation mechanisms (such as pneumatic chambers or tendons) integrate naturally into the same framework.

Finally, a structure-preserving finite element discretization leads to a finite dimensional PH system. Combined with a midpoint-based time integrator, the approach yields exact energy and momentum balance laws in discrete time, thus enhancing robustness for long-term simulations. As illustrated by numerical examples, the present framework establishes a new approach to energy-momentum consistent formulations in computational mechanics involving finite rotations.

**Reference:**

P. L. Kinon, P. Betsch & S. R. Eugster: Energy-momentum-consistent simulation of planar geometrically exact beams in a port-Hamiltonian framework. *Multibody Syst Dyn* (2025). https://doi.org/10.1007/s11044-025-10087-9

**Structure-preserving time integration of complex multibody dynamics in a port-Hamiltonian framework**

Latussek, Lisa (2,1); Kinon, Philipp L. (1); Betsch, Peter (1) 18:10

*1: Karlsruhe Institute of Technology (KIT), Germany*
*2: ETH Zurich, Switzerland*

The simulation of multibody systems (MBS), including robotic manipulators and mechanical assemblies, can be challenging due to large rotations, kinematic constraints, and complex subsystem interactions. Traditional minimal-coordinate approaches, such as Euler angles, are prone to singularities and long-term numerical instabilities.

To this end, we employ the singularity-free director formulation with constant mass matrices in a unified port-Hamiltonian (PH) framework for the simulation of rigid MBS.

The reformulation of MBS dynamics as a PH system ensures energy consistency and facilitates modularity with explicit ports for subsystem interconnection. The notion of kinematic pairs, which define ideal constraints in traditional MBS modeling, is rigorously linked to power-preserving PH interconnections, bridging conventional and energy-based perspectives.

To maintain these properties in discrete time, a structure-preserving integration based on the implicit midpoint rule is employed, additionally preventing drift-off of the position level constraints. Moreover, a modified version of the Gear-Gupta-Leimkuhler principle can be employed to obtain an index reduction of the resulting differential-algebraic equations.

As shown by representative examples, this methodology provides a modular, energy-consistent, and numerically stable approach, offering a solid foundation for control design and long-term simulation of complex mechanical systems.

## S01.02: Multi-body systems, mechatronics and robotics

Date: March 19, 2026 08:30–10:30
Room: KII, M17.51
Chair(s): Eberhard, Peter
Ebel, Henrik

### Some aspects of Small Scale Autonomous Underwater Robots for Monitoring and Manipulation in Confined Spaces

Seifried, Robert (1); Bauschmann, Nathalie (1); Grube, Malte (1); Dücker, Daniel (2) 08:30
*1: Institute of Mechanics and Ocean Engineering, Hamburg University of Technology, Germany*
*2: Munich Institute of Robotics and Machine Intelligence, Technical University of Munich*

The challenging field of autonomous small-scale underwater robotics has recently received increased attention. These systems are particularly capable of performing complex tasks in confined and cluttered environments where large-scale remotely operated underwater vehicles (ROVs) are often inefficient.

In this context, two application scenarios appear especially promising: environmental monitoring and manipulation. Applications of environmental monitoring using Autonomous Underwater Vehicles (AUVs) include radiation mapping, tracking pollutant sources, and monitoring algal blooms. These mobile robots enable dense spatial and temporal coverage at lower costs compared to static sensor networks, manual sampling, or large-scale ROVs. Furthermore, underwater manipulation is essential for tasks such as offshore maintenance, biological sampling, and hazardous material recovery. Traditionally, these operations have relied on human divers or ROVs, both of which involve high costs and operational risks. Recently, the emergence of lightweight, low-cost underwater vehicle-manipulator systems has made autonomous underwater manipulation increasingly accessible. While classical serial robot arms attached to AUVs exist, modern components from soft robotics are also being utilized. The latter are particularly advantageous for manipulating fragile objects or operating in very confined spaces. Additionally, the materials used in soft robots often have a density close to that of water, which eliminates gravity-induced static deformation—a major drawback of soft robotics on land. Although many concepts, tools, and strategies from land-based autonomous mobile robots or autonomous drones can be applied, there are also numerous unique challenges in the underwater domain.

In this talk, some of these challenges will be addressed, including modeling, localization, state estimation, control design, communication, and hardware development. Furthermore, experimental results from tests conducted in a confined test basin will be presented. While the focus is on small-scale AUVs, the presented methods are also applicable to large-scale AUVs.

### Numerical damping, overshoot and global error propagation for constrained systems

Arnold, Martin 09:10
*Martin Luther University Halle-Wittenberg, Germany*

The algorithmic damping of generalized-$\alpha$time integration methods is controlled by their damping ratio at infinity that should be strictly less than 1.0 to guarantee zero stability in the application to constrained systems. The recent convergence analysis for modified generalized-$\alpha$Lie group integrators with improved accuracy (S. Holzinger, M. Arnold, J. Gerstmayr: *$\sigma$-modified Lie group generalized-$\alpha$methods for constrained multibody systems*. - Mechanism and Machine Theory **217**(2025)106236) sparked renewed interest in the details of zero stability and global error propagation for the application to constrained systems in flexible multibody dynamics.

The global errors are considered separately for differential and algebraic solution components with a coupled error propagation that may be analysed by standard techniques from DAE numerics. The

zero stability analysis for the algebraic part relies essentially on the classical stability analysis of Newmark type integrators for a (very) stiff linear test equation (e.g., H.M. Hilber, T.J.R. Hughes: *Collocation, dissipation and overshoot for time integration schemes in structural dynamics*. - Earthquake Engng. Struct. Dyn. **6**(1978)99-117). Here, the term *overshoot* refers to an oscillating numerical solution component of large amplitude that dominates the transient behaviour but is rapidly damped out by numerical dissipation. Its equivalent in the global error analysis for the application to the index-3 formulation of constrained systems is an oscillating first order error term in the Lagrange multipliers that is damped out rapidly but deteriorates the method's second order convergence in a short transient phase after initialization or re-initialization.

The global error analysis is technically less challenging for the application of generalized-$\alpha$methods to the (stabilized) index-2 formulation of the equations of motion that considers explicitly the hidden constraints at the level of velocity coordinates. In that case, the global error propagation does not suffer from an *overshoot* phenomenon in terms of first order error terms. Global second order convergence for all solution components may be achieved straightforwardly. The corresponding mechanism of global error propagation in the algebraic solution components has again a counterpart in the classical linear stability analysis of Newmark type integrators.

**Enabling Hybrid Modeling in Commercial MBS Software: A Force-Level Approach**

Wohlleben, Meike; Linneweber, Jill Mercedes; Schütte, Jan; Sextro, Walter
*Paderborn Unsiversity, Germany*

09:30

Hybrid modeling aims to combine physical and data-driven models to increase simulation accuracy while preserving physical interpretability. In the context of dynamic mechanical systems, this enables the compensation of modeling inaccuracies that arise from simplifications, missing effects, or uncertain parameters. In this work, a hybrid model is used in which the discrepancy between simulation and measurement is learned and compensated for by a data-driven correction element. To integrate such models into commercial multibody system software like MSC Adams and Simpack, the formulation needs to be adapted to operate directly at the force level. This allows implementation via standard co-simulation interfaces without modifying the system's differential equations or solvers, thus enabling seamless integration into established industrial workflows.

Unlike previous approaches that focus on clearly identifiable components, this method addresses general model inaccuracies that cannot be assigned to specific force elements. These arise from system-wide simplifications, parameter uncertainties, or unknown physical effects, making the approach particularly suitable for complex multibody systems where traditional modeling assumptions are insufficient. The proposed force-level correction ensures that the data-driven component operates independently of the underlying numerical solver, preserving stability and compatibility with existing simulation environments.

The method is demonstrated using a three-mass oscillator with synthetic measurement data. Results show that the coupled simulation works reliably, and the hybrid model significantly improves accuracy compared to purely physical models. The correction element effectively captures unmodeled dynamics and compensates for discrepancies across the entire system, demonstrating robustness and generalizability.

**Deployment of a Finite-State Machine on a Bipedal Robot for achieving Energy-Efficient Walking Locomotion**

Mukherjee, Ashutosh (1); Luo, Yinnan (1); Zentner, Lena (2); Fidlin, Alexander (1)
*1: Karlsruhe Institute of Technology, Germany*
*2: Ilmenau University of Technology, Germany*

09:50

Recent research in bipedal robotics has increasingly targeted walking gaits that are not only dynamically stable but also energetically efficient. For underactuated bipeds, this is often achieved through the combined use of compliant drivetrain concepts and advanced feedback control strategies such as Hybrid Zero-Dynamics (HZD) control [1]. In similar efforts by the Institute of Engineering Mechanics from Karlsruhe Institute of Technology in collaboration with the Compliant Mechanisms Group from

the Ilmenau University of Technology, simulation studies of an underactuated five-segment walker under HZD control reported up to 78% reduction in energy consumption through parallel elastic couplings between the rigid segments [2]. To experimentally validate these results and evaluate the control strategy in combination with the elastic couplings under laboratory conditions, an underactuated five-rigid-segment bipedal prototype with four BLDC-Motor actuated revolute joints has been constructed, and HZD Control is implemented in real-time. The implementation follows an event-driven architecture based on a Finite-State Machine (FSM) [3].

Each walking trial starts with the prototype coming to a static and overactuated standing phase, after which it accelerates its torso segment forwards to drive the system into the stable periodic limit cycle corresponding to walking, avoiding manual perturbations to meet the required initial conditions. The FSM governs the transitions between the initial static phases to the walking phase and triggers controller resets at swing-foot impacts. Using this framework, real-time HZD Control is implemented on the prototype and walking with a prescribed walking speed and step-length is demonstrated.

**Acknowledgements:**

This work is financially supported by the Deutsche Forschungsgemeinschaft (DFG) – Project number 416912124.

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**Data-Driven System Identification of a BLDC Drivetrain for Energy-Efficient Legged Robots**

Luo, Yinnan (1); Mukherjee, Ashutosh (1); Zentner, Lena (2); Fidlin, Alexander (1)

*1: Karlsruher Institut für Technologie, Germany*
*2: Technische Universität Ilmenau, Germany*

10:10

Energy-efficient locomotion of biped robots requires actuators that are both efficient and accurately modeled. Cable-driven transmissions with brushless DC (BLDC) motors offer high energy efficiency and power density; however, they exhibit cable compliance, backlash, and nonlinearities of motor characteristics that are hard to capture analytically yet strongly influence energy consumption and control performance.

This work presents a data-driven system identification framework for a BLDC drivetrain that learns the mapping from motor current commands to output torque using experimental data, in which a single robot leg is actuated as a planar double pendulum. Two approaches are investigated and compared on the same dataset: Koopman-operator-based Dynamic Mode Decomposition [1], which provides linear predictors in a lifted observable space, and Sparse Identification of Nonlinear Dynamics with control [2], which discovers low-order nonlinear state-space models with explicit control inputs. The hardware is inspired by synthetic-fiber capstan drives for highly efficient robotic applications [3].

We summarize the experiment design and modeling workflow and show that the identified models capture key drivetrain behaviors—hysteresis, frictional effects, and current–torque nonlinearities—while remaining compact. The workflow is generic and can be applied to identify a broad class of electric drivetrains. The resulting models are directly applicable as prediction models for defining objective cost functions in trajectory optimization [4]. Moreover, the data-driven drivetrain model is integrated into a hybrid zero dynamics (HZD) control framework for legged locomotion, providing

actuator-level insight that improves torque prediction and tracking, and thereby increases the overall control accuracy of the HZD-based gait.

**Acknowledgments**
This work is financially supported by the Deutsche Forschungsgemeinschaft (DFG) – Project number 416912124.

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## S01.03: Multi-body systems, mechatronics and robotics

Date: March 19, 2026 14:00–16:00
Room: KII, M17.51
Chair(s): Ebel, Henrik
Eberhard, Peter

### Human Body Models in Real-Time Unreal Engine Physics for the Development of Safety Functions in Autonomous Vehicles

Fehr, Jörg (1); Marekar, Abhijeet (1,2); Blaume, Benjamin (2); Haringer, Matthias (2); Fahse, Niklas (1) 14:00
*1: Institute of Engineering and Computational Mechanics University of Stuttgart*
*2: VAIVA GmbH, Gaimersheim*

Safety and comfort are central enablers for emerging autonomous and distributed human-centered mobility solutions. With increasing levels of vehicle automation, interactions between humans and vehicles become more complex and less predictable, requiring robust safety functions that account for a wide range of occupants, postures, behaviors, and edge-case scenarios. Consequently, multi-scale modeling of the human—from biomechanical structure to functional and active motion—is a key prerequisite for the development and validation of future safety systems in autonomous cars.

Current automotive safety development relies heavily on high-fidelity finite-element (FE) dummy models and Human Body Models (HBMs), such as THUMS and GHBMC, which provide detailed biomechanical insight for passive safety assessment. These models are highly biofidelic and well established for crash analysis; however, they are computationally expensive and predominantly represent passive human responses. As a result, they are not suitable for real-time simulation, in-cabin monitoring evaluation, or the development of integrated active–passive safety functions. Engineers therefore lack modeling approaches that allow realistic, repeatable, and interactive evaluation of human behavior in dynamic and safety-critical pre-crash scenarios.

Recent advances in real-time physics simulation methods, graphics pipelines, and hardware capabilities—largely driven by the game industry—open new opportunities for interactive and photorealistic Digital Human Models (DHMs). This work leverages these developments by introducing a real-time surrogate digital human modeling approach implemented within the Unreal Engine physics environment, building upon industry-proven real-time simulation technology and MetaHuman character representations.

The proposed solution introduces a surrogate THUMS-based Digital Human Model that bridges the gap between established passive safety knowledge and active, human-like motion. Anthropometric

and functional human data, including joint range of motion and strength limits, are integrated to achieve realistic kinematics. Active motion is generated using reduced planar musculoskeletal models, with joint actuation represented through agonist–antagonist muscle-torque generators (MTGs), enabling physically plausible, controllable, and computationally efficient human motion in real time.

The methodology is validated by replicating experimentally established arm motion tasks, including elbow joint rotation and translational hand movements, and comparing simulation results against biomechanical reference data. Key engineering challenges addressed include coordinate system mismatches between FE-based modeling tools and the Unreal Engine environment, as well as achieving deterministic physics behavior independent of render frame rate.

The presented approach enables realistic, real-time testing of safety-critical scenarios in early development phases of autonomous vehicles, particularly for the generation of synthetic training data for occupant monitoring systems.

**Simulation of Friction-Induced Effects in Web Handling with Curved Contact Geometry**

Zeberle, Christian; Stiegelmeyr, Andreas; Heieck, Frieder 14:40
*Kempten University of Applied Sciences, Germany*

Friction is a pivotal parameter in the context of packaging goods, because it links material properties, machine design, and operational performance. This paper presents a simulation approach for modeling frictional forces between flexible web materials used in packaging technology and curved contact surfaces, based on the capstan equation. The simulation model is implemented in OpenModelica as a component-based multibody simulation model. The classical capstan formulation is extended by a state-based friction contact description, enabling the representation of sticking and sliding regimes as well as
stick–slip and slip–stick transitions.
To experimentally characterize material-specific friction behavior under realistic operating conditions and to parameterize the simulation model, a dedicated friction testing bench with a novel measurement concept was developed. The bench allows various test scenarios and enables the systematic investigation of the influence of parameters such as relative web speed and surface pressure on the coefficient of friction.
Although primarily designed for material characterization, the testing bench is also used for model validation. Validation is performed by prescribing the measured web forces upstream of the frictional contact and comparing the resulting downstream forces with simulation results. The validation demonstrates a high degree of congruence between experimental data and simulation, demonstrating the applicability of the proposed approach for flexible web handling systems.

**On implementing the Neighbored Element Method for a fast and robust Third Medium Contact**

von Zabiensky, Max; Jantos, Dustin R.; Junker, Philipp 15:00
*Leibniz Universität Hannover, Institut für Kontinuumsmechanik Germany*

Contact is a major effect in several engineering applications, whereby the computational solution can require extensive calculation effort. A fast and robust simulation approach is desired and could lead to improvements in product design. Therefor, the Third Medium Contact is a promising scheme, which enables contact of solid bodies without predefining their contact area. Instead, the void between bodies has to be discretized. This allows investigate (self-)contact problems for which the bodies are not known apriori as in the context of topology optimization, or (soft-)robotics. Previous approaches required at least quadratic ansatz functions for hexahedron finite elements and at least cubic ansatz functions for tetrahedrons. In recent works, a new regularization approach was developed, which reduced the order of the necessary ansatz functions. This is enabled by computing the gradients of deformation measures in additional nodal degrees of freedom, i.e., as additional fields of unknowns in the finite elements. Regarding the additional unknowns, we derive a special discretization for them, the Neighbored Element Method. Therewith, the additional unknowns are discretized in the quadrature points while the displacements in the nodal degrees of freedom are computed with linear finite

elements. This leads to a fast algorithm where the displacements and the regularized set of partial differential equations, i.e., the additional fields of unknowns are solved in a staggered manner.

**Friction mechanisms and coefficients in solid lubricated PA66 - Optical observation of surface dynamics**

Graf, Matthias; Thoben, Nils; Knöner, Timo 15:20
*Hochschule Emden/Leer, Germany*

Polyamide 66 without additives exhibits mechanical properties that are too weak for many structural applications. Young's modulus and yield stress can be improved by incorporating stiff glass fibers; however, this simultaneously increases the friction coefficient—an undesirable effect in mechanical components such as bearings or gear wheels. Solid lubricants, most prominently PTFE, are widely used to reduce and stabilize friction and wear. Due to environmental concerns, PTFE is under legislative pressure and is expected to be replaced.

This systematic study includes ball-on-disk experiments using different solid lubricants (e.g., graphite, ultra-high-molecular-weight polyethylene, molybdenum disulfide). While friction and wear coefficients are recorded, the interfacial dynamics during sliding are observed using a microscope camera. Synchronizing the camera's frame rate with the rotational speed of the sample enables capturing images of precisely the same surface location over time. The resulting videos reveal the formation and transport of wear particles, their agglomeration into clumps, and the extrusion of lubricants from the base material. These surface dynamics differ significantly depending on the solid lubricant employed. The optical observations can be correlated with the coefficient of friction. The friction coefficient is governed by converging running-in behavior and a quasi-stationary state. This quasi-stationary state consistently falls into one of two characteristic levels—a lower or a higher plateau—depending on the lubricant applied. A comprehensive understanding of the friction mechanisms thus offers a basis for identifying appropriate friction modifiers tailored to this specific compound.

## S02: Biomechanics

Organizer(s): Budday, Silvia *(Friedrich-Alexander-Universität Erlangen-Nürnberg)*
Holzapfel, Gerhard *(nan)*

## S02.01: Cardiovascular and electromechanical modeling

Date: March 17, 2026 08:30–10:30
Room: KII, M17.12
Chair(s): Kuhl, Ellen

### Multi-Scale Experimental and Computational Insights into Arterial Regulation After the Ross Procedure

Famaey, Nele 08:30
*KU Leuven, Belgium*

Arterial regulation is a complex process operating across spatial and temporal scales. Disturbances in this regulation are a major contributor to cardiovascular disease, the leading cause of morbidity and mortality worldwide. Current treatment strategies typically target individual scales, ranging from pharmacological agents, gene and cell therapy, and surgical repair to diet and exercise. However, the interplay across scales remains poorly understood, leaving critical questions unanswered about up- and downscale effects and the long-term impact of both pathology and treatment.

Although arterial regulation has been studied extensively from experimental and computational perspectives, most research focuses on a single scale. Molecular and tissue-level processes are often examined in vitro and over short timescales, disconnected from systemic influences and long-term dynamics. Clinical studies, in contrast, rely primarily on non-invasive measurements that provide only an aggregate view, obscuring the contribution of individual mechanisms. Tissue samples from biopsies, surgical resections, or cadaver studies offer valuable insights but represent only a single time point.

Longitudinal animal studies allow for both non-invasive measurements at regular intervals and collection of samples at different survival time points for in vitro analyses, enabling partial integration across scales. Yet, even in multi-scale, multi-temporal experimental setups, measurement techniques often require isolating small-scale phenomena from their larger-scale context. Computational modeling overcomes this limitation by inferring system responses beyond what is directly observable and preserving multiscale interactions without physical decoupling.

Here, we present a combined experimental–computational, multi-scale approach to studying arterial regulation following the Ross procedure. This is the only aortic valve replacement that restores long-term survival while preserving quality of life. In this operation, the diseased aortic root is replaced with the patient's own pulmonary root (autograft). Exposure to systemic pressure frequently leads to progressive autograft dilatation, resulting in valve dysfunction.

We investigated the Ross procedure in humans, sheep, and rats through longitudinal follow-up studies, combining in vivo imaging with in-depth tissue analyses (RNA sequencing, proteomics, histology, and mechanical testing). These analyses revealed progressive post-surgical dilatation and tissue remodeling across all scales. Using these data, we developed computational models at the molecular, microstructural, and tissue levels.

These models enabled us to design an external electrospun support for the autograft that provides sufficient mechanical reinforcement to prevent dilatation without compromising physiological compliance, thereby avoiding maladaptive long-term responses. In ongoing work, we are currently validating the use of such a support in a rat study. Our promising results show the strong potential of computational modeling in the development of treatment solutions for disturbed arterial regulation, provided that they are supported by multi-scale experimental and clinical data.

**Comparison of Finite Element Approximations for Electro-Mechanical Models of the Human Heart**

Stengel, Laura (1); Wieners, Christian (1); Krauß, Jonathan (2); Loewe, Axel (2) 09:10
*1: Institute of Applied and Numerical Mathematics, Karlsruhe Institute of Technology*
*2: Institute of Biomedical Engineering, Karlsruhe Institute of Technology*

Computational models of the human heart play a vital role in understanding cardiac function and guiding patient-specific treatment. However, modeling accuracy must be balanced with computational efficiency, especially for time-critical applications. This study evaluates two spatial discretization methods — conforming Galerkin (CG) and enriched Galerkin (EG) — in the context of electro-mechanical cardiac simulations using active strain to model cardiac contraction and Rayleigh damping to suppress non-physiological oscillations.
A realistic bi-ventricular geometry was modeled with transversely isotropic and nearly incompressible material properties. We employed a staggered scheme coupling mechani-cal deformation and electrophysiology. We compared CG and EG discretizations across multiple mesh resolutions using both linear and quadratic elements. Key metrics included cavity volumes, computational cost, and numerical robustness. CG discretization showed locking effects with coarse meshes and linear elements, negatively impacting deformation accuracy. EG mitigated these artifacts while introducing only one additional degree of freedom per element. Although EG simulations were slightly more computationally demanding, they demonstrated enhanced numerical stability and robustness without excessive damping. Both methods performed comparably in fine meshes using quadratic elements.
The enriched Galerkin method offers a favorable balance between numerical accuracy and computational efficiency for cardiac electro-mechanical simulations. In combination with active strain and Rayleigh damping, EG provides improved deformation behavior and greater numerical robustness compared to the standard CG method. These results suggest that EG is a promising approach for realistic and efficient cardiac modeling.

**Modeling Active Cardiac Mechanics: The Role of the Right Ventricle in the Left Ventricle Function**

Ogiermann, Dennis (1); Weerasinghe, Uditha (2); Perotti, Luigi E. (2); Balzani, Daniel (1) 09:30
*1: Ruhr University Bochum, Germany*
*2: University of Central Florida, USA*

Understanding cardiac function is critical to improve clinical treatment for a wide range of cardiovascular diseases. Mathematical models of the human heart serve as a vital tool in this endeavor, supplementing experimental medicine by providing a framework to test hypotheses and investigate which predictions align with experimental data. While the reproduction of pressure-volume loops remains the standard validation target for cardiac models, recent studies have shown that the resulting myocardial strains often differ even qualitatively from experimental observations, even when physiologically plausible pressure-volume loops are derived from simulation studies [1].

This discrepancy raises fundamental questions about the underlying models and a better understanding of which features are essential for studying remodeling and the progression of heart failure. As a part of an investigating this question, we analyze the influence of the right ventricle on the active mechanical function of the left ventricle. Using our extended Hill framework [2] that allows for a unified analysis of various contraction models, we explore how the transition from single-chamber to multi-chamber geometries affects a wide range of mechanical validation criteria at peak systole. All simulations were carried out using our open source cardiac multiphysics framework Thunderbolt.jl [3].

This study demonstrates how systematic geometrical and structural investigations can provide concrete guidelines for model development. By identifying how chamber interactions influence local and global mechanics, we aim to clarify the requirements for high-fidelity cardiac mechanics simulations and offer insights into cardiac function.

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**Electromechanical Computational Model of the Human Stomach**

Cyron, Christian (1,2); Henke, Maire (1); Brandstaeter, Sebastian (3); Gizzi, Alessio (4); Aydin, Roland (1,2)

*1: Hamburg University of Technology, Germany*
*2: Helmholtz-Zentrum Hereon, Germany*
*3: University of the Bundeswehr Munich, Germany*
*4: Università Campus Bio-Medico di Roma, Italy*

09:50

Health problems related to the mechanics of the stomach (gastric mechanics) are among the most important causes of morbidity in industrialized countries. Around 10% - 45% of the general population suffer from dyspepsia (difficult digestion), which seriously compromises individual well-being and economic productivity and is often linked to the motility of the stomach. At the same time, the biomechanics of the stomach still remains poorly understood, especially compared to the cardiovascular system. Currently, biomechanical modeling of the human stomach lags around one to two decades behind biomechanical modeling of the cardiovascular system.

To help close this gap between medical needs and the state of science, we present a comprehensive computational model of the motility of the stomach. It uses the finite element method (FEM) to capture the coupled nonlinear solid mechanics and electrophysiology of the stomach and can leverage patient-specific magnetic resonance imaging (MRI) data. Muscular contractions are captured by an active-strain approach and a modified Mitchell-Schaeffer model. Non-uniform mechanical and electrophysiological parameters are defined by solving several Laplace–Dirichlet problems.

Our model can reproduce essential phenomena of gastric electromechanics, including slow wave entrainment and the propagation of ring-shaped peristaltic contraction waves. Importantly, it can reproduce also pathological disorders of gastric motility.

Our model provides a powerful tool for future in-silico studies of physiological and pathological mechanisms of the human stomach. It can thereby help unravel the mechanisms of gastric diseases and develop ideas for new therapies.

**Continuously embedded sub-structures in hyperelastic materials**

Fries, Thomas-Peter; Neumeyer, Jonas; Sojer, Magdalena; Kaiser, Michael Wolfgang

*Graz University of Technology, Institute of Structural Analysis, Lessingsstr. 25/II, 8010, Graz, Austria*

10:10

A concept for embedding sub-structures—such as fibers and membranes—into hyperelastic bulk materials is proposed and generalized from [1–3]. The bulk domain is equipped with level-set functions whose isosurfaces and/or isolines represent the geometries of the embedded sub-structures. Each level-set function implicitly defines an infinite family of continuously embedded, homogenized sub-structures, one for every level set. This framework enables advanced modeling of anisotropic materials, including timber, biological tissues, layered rocks, composites, and textiles. We formulate mechanical models that resolve the physics on individual level sets and extend them consistently to the entire bulk domain [1, 2]. These sub-structure models are coupled with classical homogeneous, isotropic bulk models, yielding a new class of material models.

For numerical analysis, the bulk domain is meshed with standard higher-order elements. These elements need not align with the embedded level sets, as is characteristic of fictitious domain methods (FDMs). However, the present approach avoids the usual challenges of FDMs and has been termed

Bulk Trace FEM in [1]. Boundary conditions and numerical integration are handled as in classical FEM, with no need for stabilization. Numerical results confirm the effectiveness of the proposed substructure models across diverse contexts, achieving optimal, higher-order accuracy when solutions are smooth.

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M.W. Kaiser, T.P. Fries: Simultaneous analysis of continuously embedded Reissner-Mindlin shells in 3D bulk domains, Internat. J. Numer. Methods Engrg., **125**, e7495, 2024. DOI: 10.1002/nme.7495

T.P. Fries, J. Neumeyer, M.W. Kaiser: A new concept for embedding sub-structures via level-sets, Proceedings of the 16th World Congress on Computational Mechanics (WCCM 2024), Vancouver, Canada, 2024. DOI: 10.23967/wccm.2024.025

## S02.02: Constitutive modeling and parameter identification

Date: March 17, 2026 16:30–18:30
Room: KII, M17.12
Chair(s): Famaey, Nele

### Understanding the poro-viscoelasticitic nature of soft biological tissues through the lens of tofu

Boes, Birte (1); Holthusen, Hagen (2); Kuhl, Ellen (2,3) 16:30
*1: University of Wuppertal, Wuppertal, Germany*
*2: FAU Erlangen Nuremberg, Erlangen, Germany*
*3: Stanford University, United States of America*

Tofu is a hydrated protein gel composed exclusively of soybeans and water. Beyond its cultural relevance, nutritional value, and environmental sustainability, tofu offers a uniquely simple yet rich model system to study the mechanics of hydrated soft tissues. Despite its ubiquity, the rheology of tofu remains incompletely characterized. Here, we use tofu as a minimal benchmark system to explore the nonlinear, rate-dependent, and water-content-controlled mechanics in poro-viscoelastic solids [1]. We perform over one hundred controlled uniaxial compression tests on silken, firm, and extrafirm tofu across multiple loading magnitudes and rates. Our experiments reveal a strongly nonlinear stress–strain response, pronounced stress relaxation, and a more than ten-fold increase in peak stress with only a six percent decrease in water content. These observations highlight the extreme sensitivity of mechanical behavior to hydration, despite the otherwise identical chemical composition. To systematically extract a constitutive model from our data, we employ automated model discovery using inelastic constitutive neural networks [2]. The framework identifies inelastic constitutive laws that accurately reproduce both training and test data across three tofu types, four loading amplitudes, and five loading rates. By design, the discovered models autonomously delineate elastic and inelastic mechanisms. The elastic response is governed primarily by the second isochoric invariant. The inelastic response depends on a coupled contribution of the second and third deviatoric invariants that reflects a shear-dominated dissipation with a sensitivity to stress state asymmetry. Notably, this functional form is universal across all tofu types. Water content enters the constitutive description as a modulating feature that scales the magnitude of both elastic and inelastic mechanisms without altering their functional form. Our results demonstrate that this scaling is highly nonlinear, in contrast to the linear scaling commonly assumed in classical biphasic and poro-elastic theories. To capture this effect, we introduce a water-content-weighted feature network that embeds hydration directly into the constitutive representation. Taken together, these results position tofu as a quantitative benchmark material for nonlinear poro-viscoelasticity and demonstrate how physics-informed machine learning can uncover constitutive mechanisms in hydrated soft matter [3]. Understanding and controlling tofu rheology is essential for the reliable design of texture in alternative protein products, with implications for both human and planetary health [4]. Beyond food mechanics, our proposed

framework naturally generalizes to other hydrated soft biological tissues including articular cartilage, intervertebral discs, the cornea, the liver, and the brain.

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**Towards reliable poro-viscoelastic parameter identification with applications to human brain tissue and human meniscus**

Greiner, Alexander (1); Scherm, Philipp (1); Hinrichsen, Jan (1); Comellas, Ester (2,3); Steinmann, Paul (1,4); Budday, Silvia (1)

*1: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*
*2: Universitat Politècnica de Catalunya, Spain*
*3: International Center for Numerical Methods in Engineering, Spain*
*4: University of Glasgow, United Kingdom*

17:10

Modeling and predicting the mechanical response of multiphasic biological tissue to external mechanical loading challenges researchers since decades. The Theory of Porous Media provides a continuum mechanical framework to investigate the underlying physical mechanisms within the tissue, particularly the interactions between the deforming solid matrix and the free moving interstitial fluid. Our nonlinear poro-viscoelastic material model can capture the complex mechanical response of e.g. human brain tissue and human meniscus, but it also possesses a strong coupling between several material parameters. First, the model comprises two timescales, one controlled by the solid viscosity and one by the permeability. Second, the solid volumetric stress response governed by the first Lamé parameter affects the overall porous material response in conjunction with the deformation-dependent permeability. Therefore, it is challenging to find experimental protocols that provide all necessary information for reliable and unique parameter identification independent of the choice of initial parameters. Based on numerical experiments for three loading protocols (cyclic loading, compression relaxation and a combination thereof), we perform an exhaustive inverse parameter identification study using various sets of initial parameters and compare the results to the *a priori* known correct parameter set from the numerical experiments. Our results show that the reaction force alone does not provide enough information to reliably calibrate our poro-viscoelastic model. Especially the strong coupling between porous and volumetric effects can lead to physically unreasonable deformation states, while still providing a good but non-unique fit on the reaction force. We conduct the same numerical study again including the lateral displacement of our specimen as an additional information into the objective function of the inverse parameter identification. Our results demonstrate that including the lateral displacement significantly increases the likelihood to obtain reliable, physically meaningful parameter sets. Finally, we validate our numerical insights with actual experimental data from human brain tissue and human meniscus. We highlight the importance to record the lateral displacement during the experiment and consider it for the inverse parameter identification to accurately capture the mechanical response of biphasic tissues.

**Modelling layer- and fiber-dependent diffusion processes of extracellular vesicles in human meniscus tissue**

Nonnenmacher, Theo; Rossi, Pietro; Teixeira, Graciosa; Seitz, Andreas; Simon, Ulrich

*Universität Ulm, Germany*

17:30

[Introduction & aim]

Meniscal tears are common injuries that, due to the meniscus' crucial biomechanical role, can lead to progressive tissue degeneration and osteoarthritis. While current treatments aim to preserve or restore physiological function [1], regenerative strategies using molecular factors such as extracellular vesicles (EVs) have gained attention for their potential to enhance meniscus repair. However, it remains unclear how EVs diffuse from the synovial fluid through the meniscal layers to effectively reach resident cells. Therefore, the aim of this work was to investigate EV diffusion within meniscal tissue using a computational finite element model.

[Materials & Methods]

A three-dimensional, time-dependent, anisotropic, and spatially inhomogeneous diffusion model was established. The geometry replicates a 5-mm-thick section of the pars intermedia region of the meniscus, matching the dimensions used for excremental validation. Material properties were derived from the literature: both surface layers were modelled as isotropic with diffusivities of about 10 $\mu m^2/s$, while the central layer was assumed transverse isotropic with diffusivities of 8.5 $\mu m^2/s$ along the direction of collagen fibers [2] and 4.8 $\mu m^2/s$ perpendicular to them [3]. The initial condition was set to a concentration of 0 $mol/m^3$. Exterior boundaries were assigned a concentration of 8.3e-8 $mol/m^3$, except in one scenario where cut planes were switched to no-flux boundaries. The simulation time was 36 h with uniform time steps of 10 s for the first hour and 5 min for the remaining 35 h. A linear tetrahedral mesh (mean size 0.46 mm) was used, and spatial and temporal convergence were confirmed. Parameter variations were performed to assess sensitivity, with EV concentration at the geometric centroid serving as the primary outcome measure.

[Results]

We found that diffusion is dependent mainly on the particle size and the collagen fiber orientation in the extracellular matrix, which varies substantially across meniscal layers [2-3]. Sensitivity analysis showed that both the boundary concentration and the fiber-perpendicular diffusivity influence the centroid concentration in an almost one-to-one manner. Boundary-layer diffusivities had minimal impact, whereas fiber-parallel diffusivity exerted the strongest influence, particularly during early diffusion phases.

[Discussion & Conclusion]

The model reliably reproduces expected diffusion behavior and provides relevant insights into key factors governing EV diffusion within meniscal tissue. Both the sensitivity analysis and the no-flux cut-plane simulations highlight parameters that should be prioritized in upcoming experimental measurements. Although the model relies on combining data from various literature sources, due to the absence of experimental studies matching the exact diffusing species and anisotropic properties, this model already demonstrates the capability to deliver important results for the optimization of minimally invasive regenerative treatment strategies for meniscus.

[Acknowledgements]

This project was granted by Ulm University (Research Incubator 2025).

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**An integrated tensile bioreactor-microscopy platform for time-series observation of human articular chondrocytes under mechanical loading**

Lee, Hyun; Panitschewski, Nikolai; Navrath, Uwe; Stoffel, Marcus 17:50

*Institute of General Mechanics, RWTH Aachen University, Aachen, Germany*

Mechanical regulation of cell-mediated tissue formation remains poorly quantified due to the lack of experimental platforms that can be directly coupled with predictive mechanical models. In articular

cartilage, chondrocyte behavior is governed by local stress-strain states transmitted through the surrounding matrix, yet critical mechanical thresholds guiding phenotype transitions remain unknown. This gap limits the development of mechanistically grounded design strategies for cartilage tissue engineering and autologous chondrocyte implantation (ACI).

Knee chondrocytes exhibit mechanotransduction-driven responses accompanied by characteristic morphological adaptations that reflect cytoskeletal reorganization and local strain redistribution at the cellular scale. From a mechanics perspective, morphology provides an experimentally accessible and mechanically interpretable readout of cellular response. Because these responses are history-dependent and evolve under repeated loading, predictive, quantitative mechanoregulatory modeling requires experimental platforms capable of precisely defining mechanical inputs while enabling time-series observation of the same cell population. Importantly, mechanically driven phenotype transitions are associated with changes in the structural molecules synthesized by chondrocytes, including shifts from articular cartilage-specific type II collagen toward fibrocartilage-associated type I collagen. Such alterations in extracellular matrix composition are expected to influence tissue-scale mechanical properties, linking cell-scale mechanoregulation to emergent tissue mechanics.

Conventional approaches used to study chondrocyte mechanobiology, including endpoint molecular assays, are destructive and labor-intensive, making them poorly suited for time-resolved investigation across multiple mechanical conditions. In addition, most existing bioreactor systems separate mechanical stimulation from observation, limiting the ability to associate mechanical loading history with cellular responses within the same sample.

To address these limitations, we present an integrated tensile bioreactor-microscopy platform designed for mechanics-driven investigation of chondrocyte mechanoregulation. The system enables controlled tensile loading with repeated, non-destructive optical access to the same cell populations over extended culture durations. Tensile loading directly engages cytoskeletal stretching and adhesion-mediated mechanotransduction pathways that are difficult to isolate using compressive-only systems. The platform allows precise regulation of tensile strain amplitude, frequency, and loading duration under stable sterile culture and imaging conditions.

To enable reproducible time-series imaging, the system incorporates an automated imaging workflow based on predefined spatial coordinates and autofocus routines. Stored imaging sequences allow the system to return to identical regions of interest across time points without manual intervention. Combined with autofocus functionality, this approach enables consistent image acquisition across multiple culture wells, supporting automated, multi-well imaging and improved experimental throughput. The resulting image-based datasets provide quantitative measures of morphology evolution that serve as mechanical response proxies.

Within a broader experimental-computational framework, the controlled mechanical loading conditions established by the platform are coupled with finite element modeling to reconstruct local stress-strain fields and with data-driven approaches to identify mechanoregulatory relationships linking cell-scale responses to tissue-scale mechanical properties. By providing time-series, mechanics-consistent experimental data under well-defined boundary conditions, the proposed platform establishes a foundation for integrating experiments with modeling and simulation. Overall, this work introduces a mechanics-oriented experimental capability for systematic investigation of mechanical conditioning strategies relevant to ACI and cartilage tissue engineering.

**Parameter study of a structure to promote stiffness-driven stem cell differentiation**

Zerhusen, Lisa (1); Schätzlein, Eva (2); Weeger, Oliver (1) 18:10

*1: Technical University of Darmstadt, Cyber-Physical Simulation*
*2: Technical University of Darmstadt, Insitute for BioMedical Printing Technology*

Hydrogels have been found to be an ideal substrate for cell cultivation. Previous studies showed a stiffness-dependent differentiation behaviour of mesenchymal stem cells (MSCs). A soft matrix material with a stiffness of up to 1 kPa promotes the development of neural cells while higher stiffnesses lead to myogenic (8 – 17 kPa) or osteogenic (25 – 40 kPa) cells. Additionally, biochemical factors were used to induce differentiation [1].

This work deals with the development of a geometry that considers only stiffness-driven stem cell differentiation without the use of additional factors. The goal is to create a structure that provides a uniform and homogeneous stiffness distribution across the surface of a hydrogel poured into a PCL frame. Therefore, a parameter study of a bowtie unit cell was performed that takes not only the total stiffness into account but also its individual components.

Furthermore, a tensile testing method using a rheometer is proposed to define the hydrogel's material properties. This was found to be crucial due to the fragility of the material caused by its high water content. Due to the shear behaviour present in the rheometer tensile test, a correction factor is required. Therefore, a combination of experiments and numerical simulations has been carried out to determine hyperelastic material models for the investigated hydrogels.

[1] A. J. Engler, S. Sen, H. L. Sweeney, D. E. Discher. Matrix Elasticity Directs Stem Cell Lineage Specification. Cell 126, 677-689 (2006)

## S02.03: Vascular modeling

Date: March 18, 2026 08:30–09:30
Room: KII, M17.12
Chair(s): Linka, Kevin

### Rheological Micromechanics-Based Modeling of Human Blood as an Anisotropic Effective Medium

Massing, Florian; Müller, Wolfgang Helmut 08:30
*Technische Universität Berlin, Germany*

Cardiovascular diseases are the number one cause of death worldwide. Therefore, determination of (micro-)mechanical properties of blood is highly relevant in the field of medical technology. For instance, designing blood pumps requires knowledge about the particle deformation to prevent damaging of Red Blood Cells (RBCs), a process also known as hemolysis. Blood itself consists of white blood cells, platelets, and RBCs suspended in blood plasma, where the deformable RBCs make up the vast majority of particles. Blood plasma is sufficiently described by an isotropic, incompressible Newtonian fluid model. The particle deformation on a microscopic scale, however, is coupled to the strain-rate on a macroscopic scale. Due to this coupling, the determination of the stress-strain-rate relationship of blood as well as the concomitant particle evolution is of special interest.

There are many empirical, simplistic models available in the literature. Therefore, the model that is presented here aims at governing both the macroscopic and microscopic motion within. It is derived from established micromechanical effective medium methods. Whereas the volume fraction of RBCs in human blood is approximately *40%*, the model presented here considers blood as a suspension in the dilute limit. This serves as a building block for more complex, homogenized models that also take particle interactions into account. To derive this model, Eshelby's solution for ellipsoidal inhomogeneities exerted to homogeneous far-field conditions is used: The motion and deformation of RBCs, as well as the resulting stress contribution, are obtained by ensemble averaging over a control volume containing simplified RBCs. The resulting suspension behavior is strongly affected by the material response of the suspended particles. Therefore, different material models for the RBCs, more precisely, rigid, viscous, hyperelastic, and viscoelastic particles, are considered. In addition to the deformation and orientation of single particles, the evolution of the orientation distribution of an ensemble-averaged particle within a control volume is derived.

The analysis starts from perfectly aligned particles in a simple shear flow, and is extended to ensembles of particles in channel flows and modified geometries, such as channels with narrowing elements resembling a stenosis. First, results regarding the microscopic suspension properies, *i.e.*, the RBC deformation and orientation distribution, are presented. Second, resulting macroscopic suspension properties such as the effective shear viscosity are presented and compared to those of actual human blood.

**Exploring Atherosclerotic Plaque Progression Using a Graph-Derived Mechanochemical Framework**

Mastrofini, Alessandro (1); Tziotziou, Aikaterini (2); Bos, Daniel (2); Akyildiz, Ali (2,3); Marino, Michele (1)

*1: University of Rome Tor Vergata, Italy*
*2: Erasmus Medical Center*
*3: Delft University of Technology*

08:50

Atherosclerosis progression emerges from nonlinear interactions among lipid transport, inflammatory signaling, cellular phenotype transitions, and arterial biomechanics. While numerous computational models have provided insight into specific components of this process, integrating multiple biological and mechanical drivers within a single modeling framework remains methodologically challenging. In particular, systematically exploring how heterogeneous systemic and local inputs give rise to diverse plaque evolution scenarios across patients is still an open problem. Here, we present a preliminary application of a graph-derived mechanochemical modeling framework designed to address this gap by combining biological interpretability with multiscale spatial and mechanical modeling.

The framework originates from a curated biological interaction graph that integrates lipid species, cytokines, macrophage and smooth muscle cell (SMC) phenotypes, extracellular matrix turnover, oxidative and osteogenic cues, and mechanical drivers such as strain and shear stress. Graph edges are mapped to a coupled mechanochemical model using standardized operators, while a magnitude-based weighting scheme assigns low, medium, or high influence to regulatory interactions. This approach enables biologically meaningful modulation of pathway activity without reliance on extensive parameter tuning. Phenotype transitions, including M1 vs. M2 macrophage polarization and contractile vs. synthetic SMC switching, are represented using bistable ordinary differential equation controllers. Biochemical and cellular species evolve through diffusion–reaction partial differential equations dynamically coupled to finite-element models of arterial wall mechanics.

Simulations were conducted on two complementary geometry classes. Reduced-order synthetic geometries were generated from population-level descriptors to explore a broad range of progression behaviors, while two patient-specific carotid bifurcations were reconstructed from longitudinal imaging data. Initial and boundary conditions incorporated patient-derived blood biomarkers, including lipid and inflammatory profiles, allowing systemic inputs to directly modulate local plaque evolution.

In synthetic geometries, selective activation or suppression of graph pathways generated a wide spectrum of plaque phenotypes, ranging from lipid-dominated growth to inflammatory amplification and divergent calcification–resorption dynamics. These simulation families qualitatively reproduced patterns of variability reported in population studies. Patient-specific simulations demonstrated numerical stability and biological interpretability. Differences in LDL levels, monocyte counts, and inflammatory markers produced distinct spatial patterns of lipid accumulation, macrophage polarization, and calcification progression. Notably, local predictions of calcification growth or regression showed qualitative agreement with two-year follow-up imaging, suggesting the framework's capacity to reflect inter-patient heterogeneity even at this preliminary stage.

Overall, this work demonstrates the feasibility of a graph-derived mechanochemical framework for exploring atherosclerotic plaque progression across both population and individual scales. By integrating blood-derived inputs, spatial mechanics, and phenotype regulation within a unified and interpretable structure, the framework provides a promising foundation for future refinement toward comprehensive modeling of diverse clinical scenarios.

**A simple mechanical model of stent-vessel interaction**

Tambača, Josip (1); Canic, Suncica (2); Ljulj, Matko (1)

*1: University of Zagreb, Croatia*
*2: University of California, Berkeley, USA*

09:10

A stent is a mesh-like medical device deployed in narrowed (blood) vessels to provide mechanical support and restore unobstructed blood flow, playing a vital role in treating cardiovascular diseases.

Its long-term success critically depends on choice of appropriate stent and its precise placement, particularly in cases of asymmetric vessel occlusions.

In this work, we introduce a simplified computational model for stent-vessel interaction. The vessel is represented using the so called independent ring model, while the stent is considered as a network of elastic rods modeled as one-dimensional structure using the one-dimensional curved rod model. We establish the existence of solutions for the coupled system and demonstrate the model's applicability through numerical simulations.

## S02.04: Brain tissue testing and modeling

Date: March 18, 2026 14:00–16:00
Room: KII, M17.12
Chair(s): Ehret, Alexander E.

### Large-Strain Testing and Characterization of Brain Organoids

Scherm, Philipp (1); Reiter, Nina (1); Tranchina, Michael (2); Falk, Sven (2); Karow, Marisa (2); Budday, Silvia (1) 14:00

*1: Institute of Continuum Mechanics and Biomechanics, Friedrich-Alexander-University Erlangen-Nürnberg, Germany*
*2: Institute of Biochemistry, Friedrich-Alexander-University Erlangen-Nürnberg, Germany*

Organoids are valuable and tunable in vitro models that allow us to study the interaction between mechanics and neurodevelopment. Transient mechanical stimuli, e.g. compression, are assumed to impact organoid development by transient regulation of transcription factors and gene expression, affecting cell proliferation, differentiation, and migration. Measurements of the mechanical responses of organoids to the stimuli are currently limited to AFM while large-strain mechanics of organoids have yet to be characterized. This lack of data hinders the quantification of the organoids mechanical response, the determination of stress states experienced by cells and thus understanding of organoid mechanobiology. We aim to develop a robust testing protocol to capture and characterize the large-strain mechanical response of organoids.

Testing of organoids is impeded by their small size, inherent softness, and fragility – even more so than native brain tissue. Unconfined compression tests up to 60 % at 40 µm/s in nutritious solution using a rheometer have been performed on hiPSC-derived brain organoids. To mimic biological conditions, tests are conducted at 37°C (body temperature). Testing in fluid is necessary to avoid their desiccation and limit friction and adhesion to the testing machine. However, the measured forces are strongly affected by capillary effects, namely surface tension and Laplace pressure, that yield forces in the same magnitude as the measured force. We use simple hydrodynamic models to discriminate between the organoid and the fluid response in different testing setups and obtain the force exerted on the organoid.

Qualitatively, the results show hysteresis and a preconditioning effect similar to native brain tissue. Capturing the actual mechanical response and determining mechanical properties will aid the quantification of mechanical stimuli and their mechanobiological impact in in vitro studies.

### Mechanical Characterization of Brain Tissue Under Varied Environmental Conditions

Zhang, Hanwen; Peters, Sven; Markert, Bernd 14:20

*Institute of General Mechanics, RWTH Aachen University, Aachen, Germany*

The accurate mechanical characterization of brain tissue is fundamental for the development of high-fidelity computational models used in neurosurgical planning and injury mechanics. However, existing experimental protocols often overlook the complexities of the physiological environment. This study presents a comprehensive investigation into the mechanical behavior of brain tissue under a variety of environmental conditions. A series of mechanical tests were conducted to evaluate the sensitivity of the tissue to coupled thermal and hydration states. Subsequent constitutive modeling was performed to derive material parameters capable of capturing the observed non-linear behavior. All experiments were completed within three days post mortem to ensure tissue integrity. The results

demonstrate a significant dependency of the mechanical response on the testing environment, indicating that standard laboratory conditions may not adequately represent real tissue behavior. Furthermore, the analysis highlights the importance of accounting for specific loading modalities when determining material properties. These findings underscore the necessity of adhering to physiologically relevant protocols to ensure the validity of derived material parameters for numerical simulations.

**On direction-dependent behavior of brain tissue**

Reiter, Nina (1); Auer, Sophia (1); Hoffmann, Lucas (2); Bräuer, Lars (1); Paulsen, Friedrich (1); Budday, Silvia (1)

*1: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

*2: Universitätsklinikum Erlangen, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

14:40

Brain white matter is frequently modeled as a transversely isotropic material and recent studies have made efforts to add explicit representations of axons to microstructural models in an attempt to improve model accuracy [1]. However, measuring and explicit modeling of axons is both experimentally and computationally expensive and so far, there is no clear evidence that axons affect the mechanical behavior of the brain on the tissue or organ scale. Here, we present experimental data from multimodal mechanical testing and histological analyses of human brain white matter [2]. Results from histological analysis show that in most of the investigated regions, axons have no clear preferred direction. In the corpus callosum, where axons are most aligned, we see direction-dependent mechanical behavior, but also a strong alignment of cell nuclei and blood vessels. Since axons in the corpus callosum are comparatively thin and blood vessels are not only thicker but also stiffer than axons, we conclude that the alignment of blood vessels may cause the transversely isotropic behavior observed in the corpus callosum. Our results underline the need to investigate the effect of blood vessels on brain mechanics and provide insights on the link of brain anatomy and mechanics useful for computational modeling.

[1] Atashgar, F., Shafieian, M. & Abolfathi, N. From structure to mechanics: exploring the role of axons and interconnections in anisotropic behavior of brain white matter. Biomech Model Mechanobiol https://doi.org/10.1007/s10237-025-01957-4 (2025) doi:10.1007/s10237-025-01957-4.

[2] Reiter, N. et al. Do human brain white matter and brain stem structures show direction-dependent mechanical behavior? Acta Biomaterialia 199, 230–251 (2025).

**Modelling Brain Tssue Damage under Compressive Loading**

Goedhals, Jaime; Budday, Silvia

*Friedrich-Alexander University of Erlangen-Nuremberg, Germany*

15:00

The ultra-soft nature of brain tissue makes it susceptible to large deformations during surgical procedures, which could result in damage to the tissue. Since many neurological disorders are treated through surgery, a thorough understanding of the large-strain mechanical behaviour of brain tissue and the resulting damage are imperative. Therefore, this work presents a hyperelastic damage model for simulating damage to brain tissue. To fit the model parameters, we designed and performed dedicated compression experiments on porcine brain tissue. The combined experimental and computational modelling approach lays the foundation for the accurate prediction of brain tissue damage, during, for example, open brain surgeries, and the improvement of neuronavigation systems.

**Viscoelastic characterization of porcine brain tissue in the time and high-frequency domain**

Ruhland, Laura; Willner, Kai

*Friedrich-Alexander University Erlangen-Nürnberg, Germany*

15:20

A persistent problem in the mechanical characterization of brain tissue are inconsistent or contradicting responses, when different testing techniques are used for the characterization. Particularly challenging are techniques with varying time and length scales. However, for a mechanical model that reliably predicts the viscoelastic behavior of brain tissue under various loading conditions, it is essential to incorporate mechanical tests with varying modalities into the calibration process. This

contribution aims to address the issue of inconsistent mechanical responses when a material is characterized in different domains and to combine experimental results conducted in both the time and frequency range.

We mechanically characterized three brain areas, corona radiata, putamen and thalamus of porcine brain tissue. With a rheometer, we studied the material behavior in the quasi-static time domain under nonlinear deformations. The experiments include compression, tension and torsional shear tests in the large-strain regime under cyclical loading and relaxation. In an inverse material parameter identification, the mechanical parameters of the rheometer experiments were determined using a hyper-viscoelastic material model. For the characterization in the frequency domain, we employed magnetic resonance elastography (MRE). A tabletop MRE system measures the vibration response to shear waves induced into the tissue by a piezoelectric actuator. This method enables the acquisition of data for frequencies ranging from 300 to 2100Hz under linear deformations. The frequency-dependent material response was determined by fitting an analytical solution of the shear wave to the measured wave.

To compare the tissues time response with the frequency response, the mechanical parameters from the rheometer measurements were transformed to the frequency-dependent storage and loss modulus. Subsequently, a fractional viscoelastic material model was calibrated based on the frequency responses of both experiments. The combined study of the moduli indicates that the tissues material behavior switches from a more elastic response at low frequencies to a dominating viscosity at high frequencies. Using the calibrated model, a crossover frequency was identified at which the storage and loss modulus intersect, marking the transition from elasticity-dominated to viscosity-dominated behavior.

**Understanding In-Vivo Effects on MRE Inversion Using Full-Scale Brain Simulations**

Verma, Yashasvi (1); Heltai, Luca (2); Steinmann, Paul (1) 15:40

*1: FAU Erlangen-Nuremberg, Germany*

*2: Università di Pisa, Italy*

Magnetic Resonance Elastography (MRE) is increasingly used to characterize brain tissue mechanics *in-vivo* [1], motivating further assessment of how region-specific material properties and boundary conditions affect inversion accuracy. We present full-scale, three-dimensional *in-silico* brain MRE simulations based on patient-specific anatomy and enriched with experimentally informed *ex-vivo* material behaviour [2]. Viscoelastic properties for grey matter, white matter, and deep brain regions were assigned using frequency-dependent rheometer measurements, while cerebrospinal fluid and skull were explicitly included to capture realistic wave-structure interactions.

Shear wave propagation was simulated throughout the full brain volume under varying excitation and coupling conditions to generate synthetic displacement fields representative of MRE acquisitions. This data was post-processed using finite-difference and finite-element based direct inversion methods, enabling quantitative evaluation under controlled conditions. Reconstructed elastograms were compared to known material distributions to assess sensitivity to tissue heterogeneity, material contrast, and boundary modelling.

The results demonstrate that regional material differences and boundary interactions significantly influence shear wave patterns and reconstructed stiffness near tissue interfaces. FE-based inversions produced more convergent stiffness estimates, while FD-based methods remained computationally efficient.

[1] Hirsch, S., Braun, J., & Sack, I. (2017). Magnetic Resonance Elastography: Physical Background and Medical Applications. Wiley-VCH.

[2] Hinrichsen, J., Reiter, N., Bräuer, L. et al. Inverse identification of region-specific hyperelastic material parameters for human brain tissue. Biomech Model Mechanobiol 22, 1729–1749 (2023).

## S02.05: Muscle and endothelial tissue

Date: March 18, 2026 16:30–18:30
Room: KII, M17.12
Chair(s): Marino, Michele

### A Novel Model of Median Nerve Biomechanics and Electrophysiology in the Context of Carpal Tunnel Syndrome

Rittelmann, Jana; Bleiler, Christian; Röhrle, Oliver 16:30
*Institute for Modelling and Simulation of Biomechanical Systems, University of Stuttgart*

Carpal tunnel syndrome (CTS) is the most common entrapment neuropathy in peripheral nerves and is therefore of great importance in everyday clinical practice. CTS refers to damage to the median nerve and impairment of its function due to compression within the carpal tunnel in the wrist. One of the most prominent first symptoms is a recurring tingling sensation in the affected hands, with the motor and sensory function both declining in advanced stages.

Nerve entrapment and an increase in carpal tunnel pressure cause tissue reactions, such as swelling proximal to the compression site, and alterations in tissue properties like stiffness. The extent of the symptoms and above all the nerve damage itself is highly dependent on the severity and duration of the median nerve compression. It is essential that CTS is discovered early so that it may be reversed and further nerve damage can be prevented.

However, it is difficult to measure tissue stiffness and carpal tunnel pressure non-invasively, and there is still a need to understand the correlations between these parameters and CTS symptoms, highlighting the relevance of developing a novel model of median nerve biomechanics and electrophysiology.

Based on the anatomy and physiology of a healthy individual, a novel in-silico framework was created to investigate the mechanical behavior of the human median nerve under load. The 3D geometrical model includes the nerve's detailed microstructure considering the different collagenous layers and the axons. Individual material models based on hyperelastic strain-energy functions were formulated to account for the distinct mechanical properties of the microstructural components, including strain-stiffening behavior which is relevant in CTS diagnostics. To the author's knowledge, a model including all these aspects does not presently exist in literature.

Two finite element-based case studies were carried out, analyzing the mechanical response to longitudinal stretch and transverse compression as present in CTS. The model offers new insight into stress and stiffness distributions within nerve tissue, and provides an essential basis for future linking with electrophysiological models for signal propagation.

### Multiphysics model for the Agonist-Antagonist Myoneural Interface (AMI) integrating Continuum Mechanics and neural feedback organs

Villota-Narvaez, Yesid (1); Homs-Pons, Carme (2); Klotz, Thomas (1); Bleiler, Christian (1); Doreti, Lalith Kumar (1); Lautenschlager, Robin (3); Klink, Marian (3); Göddeke, Dominik (3); Schulte, Miriam (2); Röhrle, Oliver (1) 16:50
*1: Institute for Modelling and Simulation of Biomechanical Systems, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*
*2: Institute of Parallel and Distributed Systems, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*
*3: Institute of Applied Analysis and Numerical Simulation, Stuttgart Center of Simulation Science (SC SimTech), University of Stuttgart, Germany*

Motor control relies on the coordinated interplay of cortical drive (i.e., from the brain) and proprioception (i.e., from the body). Although amputations unavoidably limit human motion, intact neuromuscular function remains crucial for mitigating phantom pain and restoring motor function through

human-machine interfaces. Yet, restoring proprioception in individuals with limb loss remains a significant challenge because, in traditional amputation techniques, agonist-antagonist muscle pairs are severed and left as independent functional units. The Agonist-Antagonist Myoneural Interface (AMI) addresses this issue by preserving the mechanical coupling between agonist and antagonist muscles through a tendinous structure. However, the optimal pre-stretch of the tendinous structure remains unknown and is currently based solely on the surgeon's experience. To address this shortcoming, this work presents a multiphysics and multiscale simulation framework that integrates muscle control through spinal motor neurons, the electrical activation of muscles, a continuum mechanical musculoskeletal model, and neural feedback induced by sensory organs, such as Muscle Spindles and Golgi Tendon Organs (GTO). These sensors are spatially distributed and translate local mechanical states into discrete afferent firing rates, which are then integrated by the motor neuron pool to ultimately update the neural drive to the muscle. Thereby, one key methodological contribution of our framework is the coupling of substantially different classes of models. In detail, while the mechanical state (fiber strain, strain rate, and tendon tension) and the electrical state (extracellular potential) of the muscle are modeled as PDEs discretized by means of the finite element method, motor neurons and sensory organs are represented by systems of ODEs. In our work, coupling is achieved via the coupling library preCICE, which is designed for partitioned multi-physics simulations and is capable of coupling different solvers with a minimally invasive approach. To showcase the physiological plausibility of the proposed model, we implemented an isometric setup of a severed limb with immobilized bones. In this condition, the activation of the agonist only produces tension on the shared tendon and stretches the antagonist. We simulated active contraction of the agonist muscle, and tested the influence of muscle pre-stretch on the firing signal of the reflex organs. In summary, this work presents, for the first time, a simulation framework that couples motor control and musculoskeletal mechanics through a realistic physiological-system model. We anticipate that this model can be used in the future to guide surgical procedures aimed at optimizing proprioception recovery in amputation patients.

**Revisiting active skeletal muscle tissue: An inherently-stable, continuum-mechanical constitutive formulation with history dependence**

Bleiler, Christian; Röhrle, Oliver 17:10
*Institute for Modelling and Simulation of Biomechanical Systems, University of Stuttgart, Germany*

The force-length relationship is a fundamental ingredient for active skeletal muscle models. However, it originates from isometric experiments and does not inherently predict the mechanical behaviour during active lengthening or shortening. While this limitation is well known, it is frequently bypassed in practice. To mitigate the resulting stability issues on the descending limb, sophisticated strategies have been developed, most notably the active-stretch approach based on the multiplicative decomposition of the deformation gradient. This has led to a persistent debate regarding the superiority of active-stretch versus active-stress formulations.

In this work, we revisit the observation that the perceived instability of the descending limb can be naturally resolved by accounting for the contractile history of the tissue. We demonstrate that by incorporating these history-dependent effects, the constitutive response becomes inherently stable during active stretching without requiring additional numerical remedies. We propose a straightforward model based on the additive composition of passive elastic and active (pseudo) potentials. This formulation is conceptually aligned with the active-stress approach, providing a simpler yet robust alternative for simulating complex muscle dynamics.

By ensuring a stable and physically consistent response during active deformations, this approach enhances the reliability of stress predictions, also in scenarios such as eccentric loading, which is crucial for injury prediction and possible clinical applications. Due to its phenomenological formulation with a minimal set of parameters, the model is particularly well-suited for large-scale musculoskeletal simulations and offers a robust and computationally efficient framework.

**A Simulation Framework for Force Transmission in the Muscle Fiber-Endomysium System**

Doreti, Lalith Kumar (1); Danesini, Paolo Carlo (2); Villota-Narvaez, Yesid (1); Bleiler, Christian (1); Ates, Filiz (2); Röhrle, Oliver (1)

*1: Institute for Modelling and Simulation of Biomechanical Systems (IMSB), University of Stuttgart*
*2: Institut für Statik und Dynamik der Luft- und Raumfahrtkonstruktionen (ISD), University of Stuttgart*

17:30

Force transmission in skeletal muscle involves complex interactions between muscle fibers and the endomysium, the surrounding connective tissue. While these mechanisms hold significant clinical relevance in the treatment of musculoskeletal diseases, experimental validation remains technically challenging. Consequently, computational modelling has become an attractive and essential tool for hypothesis testing and mechanistic understanding. This study develops a simulation framework to explore the force transmission in the muscle fiber-endomysium system. The integrated system uses an isotropic, hyperelastic, nearly incompressible formulation, specifically the Demiray model, to represent the passive material behaviour. Additionally, a sigmoid-type activation function is incorporated to simulate the muscle fiber's active behaviour. The material properties of passive structural elements and the active part are fitted to experimental data obtained from muscle fibers of the extensor digitorum longus (EDL) of Wistar rats, ensuring biological relevance. Using finite element simulations, we systematically investigated how connective tissue affects the transmission of both the active and passive force in the muscle fiber-endomysium system. We compare passive and active force in simulations with intact and dissected endomysium between muscle fibers. Thus, the computational framework developed in this study enables systematic exploration of biomechanical hypotheses that would be prohibitively difficult to validate experimentally.

**Multi-phase field approach to modeling the fracture behaviour of smooth muscle tissues**

Deo, Rohan Hemant (1); Liu, Jintian (1); Siebert, Tobias (2); Böl, Markus (1)

*1: Institute of Mechanics and Adaptronics, Technical University Braunschweig, Braunschweig, Germany*
*2: Institute of Sport and Movement Science, University of Stuttgart, Stuttgart, Germany*

17:50

Smooth muscle (SM) tissue is a crucial component of the involuntary muscle system and plays an important role in the functional activities of hollow organs, such as blood vessels, the small and large intestines, the urinary bladder, the stomach and the uterus. Here, it sustains extensive deformation while preserving mechanical integrity. The functionality of SM tissue is primarily governed by its key components: elastin, collagen and smooth muscle cells (SMCs). These components are arranged non-uniformly within the different layers of hollow organ walls and have distinct mechanical characteristics and microstructural orientations. To address fracture-related pathologies in SM tissue effectively, numerical simulations are performed to study the failure behaviour of these individual components and their impact on overall organ function and potential pathologies. To this end, a novel three-dimensional, multi-phase field framework has been developed to model fracture mechanisms in SM tissue. This approach uses independent phase field damage descriptors to represent the failure of each major component, enabling the investigation of component-specific fracture behaviour within SM tissue. To achieve a more realistic representation, the model incorporates the anisotropic elastic and fracture behaviour of fibrous components, as well as their compositional heterogeneity, which is observed in different SM tissues and often reflects the specific functionality of hollow organs. The model's versatility is demonstrated by numerical simulations performed on tissue strips, including uniaxial loading and varying fracture-related material properties. While conventional single phase-field models capture the failure behaviour of the overall (homogenised) wall of the hollow organ, the proposed multi-phase field approach provides a robust computational tool for investigating fracture initiation and propagation within the multiple components (elastin, collagen and SMCs) of SM tissue under diverse physiological and pathological conditions.

**A computational model to rationalize endothelial damage under acute loads**

Ehret, Alexander E. (1,2); Jakob, Raphael (2); Giampietro, Costanza (1,2); Mazza, Edoardo (1,2) 18:10

*1: Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland*

*2: ETH Zurich, Institute for Mechanical Systems, 8092 Zürich, Switzerland*

The endothelium - a single layer of cells - covers the luminal surfaces of blood and lymph vessels. It represents the first selective barrier between these body fluids and the soft surrounding tissues, and takes a key role in controlling the transport of immune cells and molecules between them. Various diseases and pathologies are related to a loss of endothelial integrity, causing impaired barrier functions. Here we consider damage of the endothelium due to acute, i.e. high and rapid mechanical loads as they can occur during cardiovascular medical interventions.

Recent studies have shown that the endothelium in different states, also related to age, shows different fracture patterns, mainly differing in the localization of the damage within or in between cells. Related to this is a different capacity of re-establishing monolayer integrity over time by closing the gaps [1]. Moreover, we showed experimentally that the amount of damage strongly depends on the kinematic load state [2]. These observations were analyzed by means of a recently developed custom discrete network model of the endothelium accounting for cytoskeletal fibres and their failure [2,3]. The simulations allowed rationalizing the experimental data, thus qualifying the model as a valuable tool to study endothelial damage [1-3], and thus as a means for the computational analysis of corresponding problems in cardiovascular medicine.

In addition to highlighting these results, the present contribution focuses on the theoretical background and computational technique developed to model damage and fracture in the large, generally sub-isostatic cytoskeletal fibre networks by use and adaption of methods from molecular dynamics.

**References**

[1] Choi Y. et al. (2024) Biomater. Adv. 163:213938, doi: 10.1016/j.bioadv.2024.213938.
[2] Jakob et al. (2025) Acta Biomater. 207:380–397, doi: 10.1016/j.actbio.2025.09.041
[3] Jakob et al. (2024) Biomech. Model. Mechanobiol. 23:941-957, doi: 10.1007/s10237-023-01815-1

## S02.06: Orthopedics

Date: March 19, 2026 08:30–10:30
Room: KII, M17.12
Chair(s): Budday, Silvia

**Advanced computational models of human extremities to improve medical evidence in total knee arthroplasty**

Avci, Okan; Ranjan, Animesh; Yildiz, Armagan Can 08:30

*Fraunhofer IPA, Germany*

More and more young patients with knee pain such as osteoarthritis are undergoing total knee arthroplasty (TKA) worldwide. However, the risk of implant revision in young patients is much higher than in older patients. Obviously, they are more active and mobile than older patients and therefore the loads on the implant and the musculoskeletal system are higher. According to statistics in Germany, the risk of first implant failure after two years is twice as high in the patients under 55 years than in the age group above 65 years. Misplacement and misalignment of the implant relative to the biomechanics of the joint may be one of the critical factors. The position of the implant in the knee is currently determined geometrically using static medical imaging data of the bone anatomy. However, the effects of alignment and the functional constraints and limitations of implants on the musculoskeletal system are not fully understood. If the biomechanics of the joint system is disturbed and overstressed by the implant and/or surgery, it will lead to muscle imbalance and unnatural movements.

Our motivation is to overcome these problems through in silico studies. We are developing human models that accurately represent the 3D musculoskeletal anatomy and physiology of joints in a realistic way through continuum mechanical tissue models of the muscle tendon unit (MTU). I will present

a novel approach to optimise the internal stretch or pre-stretch of the MTU within a musculoskeletal system based on a given range of motion ratio, which is important for maintaining muscular balance in the joint system. Without muscle pre-stretch, active motion of the extremities would be almost impossible. Moreover, this optimisation scheme also enables us to incorporate muscular disorders into the musculoskeletal system to create a cohort of virtual patients.

In this regard, I will present our latest developments on the In Silico Human Modelling (ISHM) platform. These range from medical imaging to complex 3D biomechanical simulations of the musculoskeletal system, which are performed using the finite element method (FEM). I will also present a practical application of our current research work with an industrial partner. The in silico study evaluates the functional and biomechanical performance of TKA for bone tumours. This novel analysis reveals differences in knee kinematics between a knee joint replacement and a physiological knee joint stabilised only through connective tissues and MTU. The study also analyses aspects related to joint replacements with fixed and mobile bearings, as well as the impact of surgical misalignment of the implant on knee joint motion. The results of this ongoing study will inform future implant navigation strategies for surgeons and the design of the next generation of patient-specific implants.

**Adaptive and Predictive Digital Twins in Orthopaedics: A Multimodal Patient-Specific Approach**

Andres, Annchristin (1); Roland, Michael (1); Braun, Benedikt (2); Diebels, Stefan (1) 08:50

*1: Universität des Saarlandes, Angewandte Mechanik, Saarbrücken Deutschland*
*2: Klinik für Unfall- und Wiederherstellungschirurgie, Eberhard Karls Universität Tübingen, BG Klinik Tübingen, Tübingen, Deutschland*

The ongoing digitization of medicine is opening up new perspectives for patient-specific modeling, simulation, and prognosis of orthopedic healing processes. This study presents a unique database built up over five years that includes patients with fractures of the long bones of the upper and lower extremities (tibia, femur, radius, and humerus). The database currently contains 100 fully documented cases, based on a standardized, specially developed workflow (1).

Each data set includes multimodal information, including imaging data (CT images, X-ray), motion analyses using the Xsens$^{TM}$ motion capture system, and musculoskeletal simulations using AnyBody$^{TM}$ software. For patients with fractures of the lower extremities, the team additionally recorded ground reaction forces using instrumented soles. Andres et al. (2) describe the methodological principles and technical capabilities of these combined measurement systems.

Based on this data structure, the creation of digital twins for orthopedic-traumatological applications was established (3). This human digital twin approach enables patient-specific mapping of biomechanical analyses and the simulation of individual stress scenarios. In addition, these models can be used to predict healing processes and provide quantitative support for therapy decisions. For example, the workflow enabled prediction of the effects of individual partial loads on mechanical stability and healing progress in tibial head fractures (4).

The database presented here thus provides a basis for developing adaptive and predictive digital twins, which are highly relevant to both research and clinical decision-making. By linking imaging, motion data, and biomechanical simulation, patient-specific factors influencing fracture healing can be systematically analyzed and quantified. In addition, the database opens new possibilities for the use of machine learning and artificial intelligence methods, particularly for automated classification, pattern recognition, and the prognosis of individual healing processes.

This unique data basis thus represents an important step toward data-driven, personalized orthopedics and trauma surgery. In the future, it will be continuously expanded and supplemented with additional measurement methods to further improve the precision of digital twins and open new clinical fields of application.

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4. Andres A, Roland M, Wickert K, Diebels S, Truhn D, Histing T, et al. Predicting the effect of individual weight-bearing on tibial load and fracture healing after tibial plateau fractures–introduction of a biomechanical simulation model. Front Bioeng Biotechnol. 2025;13:1–13.

**Physiological strain windows driving fracture healing: a simulation-based framework for site-specific modeling**

Roland, Michael (1); Andres, Annchristin (1); Diebels, Stefan (1); Tjardes, Thorsten (2)

*1: Applied Mechanics, Saarland University, Saarbrücken, Germany*
*2: Hospital of the German armed forces Berlin, Berlin, Germany*

09:10

Fracture healing is governed by mechanobiological regulation, in which local mechanical stimulus is the primary driver of cell differentiation, tissue formation, and remodeling in the callus. Existing mechanobioregulatory models and Frost's mechanostat define strain "windows" for healing and bone formation but thresholds mainly come from animal lower-limb data and are poorly specified across human bones and anatomical sites. Because loading and mechanosensitivity are site-specific, it is unclear whether strain ranges at one region can be transferred to others without bias. We hypothesize that the strain window for bone formation in fracture callus corresponds to Frost's physiological usage window at the same anatomical site, and that this relationship can be quantified via simulations.

We constructed subject-specific finite element models of healthy and fractured long bones (lower and upper extremity) based on clinical imaging. Physiological activities (walking, stair negotiation, and a palm-leaning task) were applied using musculoskeletal simulations based on motion capturing data to estimate joint and muscle forces. For healing scenarios, callus tissue was represented by time-varying material properties and mechanobioregulatory rules adapted from literature models. For each site and activity, distributions of different strains were quantified. The strain-states were then compared to the corresponding physiological usage windows.

Across all subjects and activities, the peak and median strains in the regions of bone formation were within the callus or only slightly deviated from the physiological usage window derived for the corresponding healthy bone site. In addition, for the different bones considered and the different probands, there was also an inter-individual strain variability observable.

Our simulations support a quantitative overlap between the physiological usage window and the strain ranges that drive osteogenesis in fracture healing at matched anatomical sites. This linkage can provide a pathway to generate mechanically driven site-specific differentiation rules.

**ML-based porous metamaterial design for hip implant stability and bone growth**

Aldakheel, Fadi (1); Haertlé, Marco (2); Ayouch, Badr (1); Eimke, Laurenz (1); Antonini, Alberto (1)

*1: Leibniz Universität Hannover, Institute of Mechanics and Computational Mechanics, Hannover, Germany*
*2: Hannover Medical School, Orthopedic clinic, Hannover, Germany*

09:30

Despite major advances in biomaterial compatibility, medical implants still exhibit failure rates that remain high compared to technical systems, largely due to limited understanding of biophysical integration processes, such as bone growth and implant stability. While high-fidelity computational models can provide valuable insights, their computational complexity and cost hinder patient-specific analyses and limit clinical adoption.

This contribution presents a machine learning–based inverse design framework for porous metamaterials targeting hip implant stability and bone growth. By combining finite element simulations with real clinical data, surrogate models are developed to efficiently relate microstructural features to effective mechanical and transport properties. In particular, a deep generative property-variational

autoencoder (pVAE) framework is developed to enable inverse design of porous microstructures with implant-relevant target properties.

Overall, the approach offers a scalable pathway toward patient-specific implant assessment and design, with the potential to support future clinical decision-making.

**Multiphysics phase-field modelling of stress corrosion cracking in PEO-coated biodegradable magnesium alloys**

Zhang, Dawei; Ma, Sonyun; Markert, Bernd 09:50
*Institute of General Mechanics, RWTH Aachen University, Germany*

Biodegradable magnesium alloys have emerged as highly promising biomaterials for temporary orthopaedic implants due to their ability to degrade naturally within the human body. This property eliminates the need for secondary surgical procedures, which reduces patient discomfort and alleviates the burden on healthcare systems. However, a high corrosion rate may cause premature implant failure under physiological conditions. To address this issue, plasma electrolytic oxidation (PEO) treatments have been extensively investigated to control the corrosion rate. However, the PEO coatings are typically porous and contain numerous micro-defects, which permit electrolyte penetration into the alloy substrate during immersion. This significantly compromises the protective efficacy of the coatings and exacerbates their degradation, particularly when subjected to external mechanical loadings. Consequently, a deep understanding of the degradation behaviour of PEO-coated magnesium alloys is essential for their successful application in biomedical implants.
This study presents a multiphysics phase-field model to capture the interactions among corrosion, fracture, and hydrogen diffusion associated with the stress corrosion cracking phenomena. The proposed model incorporates displacement field, fracture field, corrosion field, magnesium concentration field, and hydrogen concentration field as global primary variables. The model is validated against in vitro experimental data, and quantitative computational analyses are conducted to investigate the effects of PEO coatings and environmental factors on the degradation processes of coated magnesium alloys.

**Digital-Skin-Twin: In-Silico Planning for Personalised Skin Laser Treatment**

Seyedpour, Seyedmorteza (1,2); Azhdari, Mohammad (1); Rezazadeh, Ghader (3,4); Tautenhahn, Franziska (5); Tautenhahn, Hans-Michael (6); Ricken, Tim (1,2) 10:10
*1: Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Pfaffenwaldring 27, Stuttgart, 70569, Germany*
*2: Porous Media Lab, Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart , Pfaffenwaldring 27, Stuttgart, 70569, Germany*
*3: Center for Materials Technologies, Skolkovo Institute of Science and Technology, Moscow, Russia*
*4: Mechanical Engineering Department, Faculty of Engineering, Urmia University , 11km Sero Road, Urmia, 16557153, Iran*
*5: Experimental Hepatobiliary Surgery Group, Department of Hepatobiliary Surgery and Visceral Transplantation, Liebigstraße 20, Leipzig, 04103, Germany*
*6: Department of Oral, Maxillofacial and Plastic Facial Surgery, University of Leipzig Medical Center, Liebigstr. 12, Haus 1, Leipzig, 04103, Germany*

Uncontrolled laser penetration into the deeper layers of the skin, particularly the reticular dermis, can result in thermal injury, including burns, tissue necrosis, and hypo or hyperpigmentation. Despite substantial progress in dermatological laser therapies, the overall architecture of laser-based dermatology systems has undergone limited true innovation aimed at resolving the fundamental challenges of the field. Most of the existing developments have focused on incremental adjustment of individual parameters rather than the introduction of new systemic mechanisms. The objective of this study is to propose a novel mechanism for laser-based skin therapy that addresses critical issues such as damage to superficial and surrounding tissues and the need for precise control of laser penetration depth. To this end, a multi-beam laser configuration—potentially incorporating different dermatological laser types, is modelled in combination with an impinging jet for surface cooling. The resulting heat-transfer data from these simulations are subsequently used to train a neural network, which is

employed to elucidate the relationships between multiple system parameters and the corresponding thermal response, thereby enabling parameter optimisation for specific therapeutic applications. Based on these findings, the practical design, construction and implementation of this mechanism as a medical device are analysed and evaluated for feasibility. The results of the simulation and modelling indicate that the proposed mechanism can be highly effective for selective therapies targeting specific skin tissues or regions. Furthermore, by training the neural network on a medical-device configuration, treatment parameters can be individualised for different patients. Although this approach may increase the cost of dermatological procedures, its advantages relative to conventional techniques are considered sufficient to justify its adoption.

## S02.07: Growth and microorganisms

Date: March 19, 2026 14:00–16:00
Room: KII, M17.12
Chair(s): Röhrle, Oliver

### SynGROW – A novel framework for the Synthetic Generation of Rigorously Optimized Volumetric Vasculature

Jessen, Etienne (1); Steinbach, Marc C. (2); Schillinger, Dominik (1) 14:00
*1: Institute for Mechanics, Computational Mechanics Group, Technical University of Darmstadt, Germany*
*2: Institute of Applied Mathematics, Algorithmic Optimization Group, Leibniz Universität Hannover, Germany*

Functional assessment of organs is essential for improving treatment strategies. Detailed knowledge of an organ's vasculature can significantly enhance this assessment and advance our understanding of vascular development. However, existing approaches for synthetic vascular generation often rely on restrictive modeling assumptions, local optimization schemes, or computationally expensive algorithms.

Building on our previous work [1–3], we introduce SynGROW, a framework for the rapid generation and analysis of hierarchical vascular trees based on global optimization. SynGROW can simultaneously optimize multiple non-intersecting trees, yielding realistic vessel curvature and tortuosity, while achieving at least an order-of-magnitude speedup over state-of-the-art methods [4].

We demonstrate the capabilities of SynGROW through full-scale reconstruction of the cerebral microcirculation in a human brain. The generated vasculature reproduces key transitional features between pial and penetrating vessels in the cortical region [5], highlighting the framework's ability to capture anatomically meaningful vascular organization.

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**A multiscale-multiphysics framework for modeling organ-scale liver regrowth with quantitative validation after 70% partial hepatectomy in mice.**

Hohl, Jannes; Jessen, Etienne; Schillinger, Dominik 14:20
*Technical University of Darmstadt, Germany*

Liver regeneration after partial hepatectomy is tightly coupled to post-operative hemodynamic perturbations: resection induces organ-scale hyperperfusion, which initiates growth and vascular remodeling until a homeostatic perfusion state is re-established. Building on our previously introduced framework for modeling liver regrowth on the organ scale [1], we present a validation study in mice after 70% partial hepatectomy (PHx).

The modeling framework is based on three components: (1) a multiscale perfusion model that combines synthetic vascular tree generation with a multi-compartment homogenized flow model, including a homogenization procedure to obtain effective parameters; (2) a finite growth model that acts on all compartments and the synthetic vascular tree structure; and (3) an evolution equation for the local volumetric growth factor, driven by the homogenized flow rate density through the microcirculation as a measure of local hyperperfusion and well-suited for calibration with available data. The microcirculatory resistance is linked to representative lobule-level computations, allowing micro-scale physics to inform organ-scale response.

Murine 70% PHx is a particularly stringent and well-controlled validation setting because the mouse liver is partitioned into distinct macroscopic lobes, enabling reproducible resections that typically remove entire lobes and yield a well-defined remnant geometry and boundary-condition shift. In the standard 70% PHx protocol, the median and left lateral lobes are ligated and resected, removing approximately 70% of total liver mass [2]. We calibrate our model and validate it against time-resolved experimental data at three complementary levels: (i) organ-scale regrowth (liver mass and shape), (ii) global hemodynamics (portal pressure and flow rates), and (iii) regional perfusion across the remnant lobes. We will report the calibration strategy and validation outcomes, including where the model is consistent with data and where discrepancies indicate missing mechanisms.

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**Finite growth of N-phase mixtures: a thermodynamically consistent Lagrangian framework with application to avascular tumor growth**

Stollberg, Jonathan; ten Eikelder, Marco F. P.; Schillinger, Dominik 14:40
*Institute for Mechanics, Computational Mechanics Group, TU Darmstadt, Germany*

Mixture theory and finite growth mechanics have proven effective for describing biological systems in which multiple constituents interact, exchange mass, and undergo growth-driven deformation. Motivated by these developments, we formulate a thermodynamically consistent framework for N-phase growing mixtures within a fully Lagrangian setting. A key feature of the approach is the multiplicative decomposition of the deformation gradient of a solid skeleton, which allows growth to be clearly distinguished from elastic deformation. Starting from the balance laws of mass and momentum for each phase, we impose the local dissipation inequality to restrict admissible constitutive behavior. This leads to a systematic derivation of constitutive relations for the free energy, growth kinetics, and interphase mass exchange. As a result, we obtain coupled evolution equations for the phase fields and their associated chemical potentials that are consistent with the second law of thermodynamics and suitable for modeling a broad class of growth processes.

To illustrate the capabilities of the framework, we apply it to the modeling of avascular tumor growth. The tumor is treated as a saturated mixture composed of multiple solid tumor cell populations and

interstitial fluids. By selecting specific free-energy functions, growth laws, and source terms, we capture key biological mechanisms such as cell proliferation, competition between cell populations, and nutrient-limited growth. The resulting model consists of a strongly coupled system of equations that is well suited for numerical simulation.

**Microbial modelling of the growth of microorganisms and biological production kinetics**

Liu, Qiyue (1); Kozanecka, Zuzanna Justyna (2,3); Liu, Jintian (1); Krull, Rainer (2,3); Böl, Markus (1,3) 15:00

*1: Institute of Mechanics and Adaptronics,Technical University Braunschweig,Braunschweig, Germany*
*2: Institute of Biochemical Engineering,Technical University Braunschweig,Braunschweig, Germany*
*3: Center of Pharmaceutical Engineering(PVZ), Technical UniversityBraunschweig, Braunschweig, Germany*

The filamentous actinomycete *Actinomadura namibiensis* is attracting increasing interest due to the production of the secondary metabolite *labyrinthopeptin A1*, which exhibits broad spectrum antiviral activity against HIV, HSV, Zika and Dengue viruses. As the sole known natural producer, *Actinomadura Namibiensis* and its application in the cultivation process have been characterised experimentally. In order to gain a deeper understanding of the process factors and enhance productivity efficiently, microbial modelling is required to describe the underlying mechanisms, enabling numerical prediction of the cultivation process and target optimisation. For the formation of secondary metabolites, the supply of oxygen of the pellets is crucial and is closely coupled with the consumption of various resources.

To address this, a pellet-level diffusion-reaction model has been developed to quantitatively describe nutrient uptake, growth, maintenance metabolism, and oxygen transport within a spherical fungal pellet. This allows product titers to be estimated under different process conditions. The model couples the consumption kinetics of glucose and glycerol with pellet growth and maintenance metabolism, taking into account oxygen transfer limitations and the diffusion behaviour impacted by the growth-induced volumetric changes. The model parameters are identified using an inverse approach based on experimental results obtained at different scales: Substrate consumption and dissolved oxygen concentration are monitored and simulated at pilot scale, while a pellet-level oxygen profiling experiment is simulated with different boundary conditions. Good agreement was revealed when the experimental and simulated results were compared at both scales and on different cultivation days.

This study provides a detailed mechanistic understanding of nutrient uptake and mass transfer limitations within the fungal pellets, establishing a foundation for the quantitative prediction of productivity and providing a modelling framework for similar filamentous microorganisms. By resolving the cultivation process and associated mechanisms at pellet and pilot scales and linking measurable signals to model variables, the proposed approach enables interactions between mass transfer in filamentous microorganisms, metabolic activity and production kinetics to be interpreted more reliably. Furthermore, the model calibration and the corresponding experimental design proposed in this study can be applied to a wide range of other microorganisms, cultivation systems and even upscaling optimisation studies for industrial biotechnology.

**Novel hybrid simulation approach for filamentous microorganisms with multi-material populations in bioprocesses**

Kardooni, Mohammad Reza (1); Kozanecka, Zuzanna Justyna (2); Liu, Jintian (1); Krull, Rainer (2); Böl, Markus (1) 15:20

*1: Institute of Mechanics and Adaptronics, Technische Universität Braunschweig*
*2: Institute of Biochemical Engineering, Technische Universität Braunschweig*

The productivity of labyrinthopeptin A1 as a highly promising antiviral compound depends strongly on the cultivation of filamentous microorganisms and the processing conditions. The mechanical interactions in shaken cultivation systems play an important role in the morphological evolution of microorganisms, and consequently in mass transfer and process productivity. To numerically predict contact behaviour and turbulent behaviour, the microorganisms are modelled as spherical pellets,

and a hybrid CFD-DEM-VOF framework is proposed to quantify pellet-pellet and pellet-wall interactions. Given the wide range of physical properties, the pellets are assigned specific sizes, densities, and mechanical stiffness. This enables the calculation of contact forces, collision frequencies, and kinetic energy levels within the resolved hydrodynamic field. The framework is parameterised using experimental results obtained at different stages of cultivation, enabling the analysis of contact and shaking behaviour. Furthermore simulations under various conditions reveal that agitation intensity and the mechanical properties of the pellets strongly influence their interactions, beyond changes arising from natural culture development. Overall, the framework establishes a mechanistic link between operating conditions, pellet restructuring and bioprocess performance, enabling predictive process design.

**On the mechanical behaviour of grass structure for coastal protection**

Klaus, Katja (1); Liu, Jintian (1); Schürenkamp, David (2); Goseberg, Nils (2); Böl, Markus (1)

*1: Institute of Mechanics and Adaptronics, Technical University Braunschweig, Braunschweig, Germany*
*2: Leichtweiß-Institute for Hydraulic Engineering and Water Resources, Technical University Braunschweig, Braunschweig, Germany*

15:40

Coastal vegetation provides protection against erosion and wave attenuation in coastal areas. However, rising sea levels, caused by climate change are altering the propagation speed and kinetic energy of waves near the coastlines, reducing the effectiveness of this natural protection system. To quantitatively assess the contribution of coastal grass to wave attenuation, this study investigates the mechanical behaviour of *Elymus species* and proposes a material model capable of estimating mechanical responses under various conditions within the fluid–structure interaction framework. Unlike previous studies, which have performed bending experiments to characterise the mechanical behaviour of*Elymus*, this study considers mechanical behaviour under different deformation states and the contribution of nodes to the bending resistance of the whole stem. This aims to achieve a more accurate estimation of the mechanical responses of the*Elymus* structure. To this end, the structure of the nodes was investigated through histological analysis, while their elastic material behaviour was examined using an inverse approach based on the structural behaviour obtained under different loading conditions. Combining the structural reconstruction of the nodes and internodes with their corresponding material properties reveals the nodes' obvious contribution to bending resistance. This enhancement enables more accurate prediction of the bending configuration under flow- and wave-induced loading conditions.

## S03: Damage and fracture mechanics

Organizer(s): Tsakmakis, Aris *(Technische Universität Darmstadt)*
Ricoeur, Andreas *(Universität Kassel)*

## S03.01: Concrete

Date: March 17, 2026 08:30–10:30
Room: KII, M17.74
Chair(s): Aldakheel, Fadi

### Modeling Corrosion-Fatigue Degradation in Reinforced Concrete Structures

Gopakumar, Manikandan; Kenjo, Ghandi; Baktheer, Abedulgader; Aldakheel, Fadi 08:30
*Institute of Mechanics and Computational Mechanics, Leibniz Universität Hannover*

The interaction between corrosion and fatigue represents a highly complex, strongly coupled chemo-mechanical degradation process that critically affects the durability of reinforced concrete structures exposed to chloride-rich environments and cyclic loading. Corrosion of steel reinforcement induces cracking and loss of cross-section, increasing stress concentrations and accelerating fatigue damage, while fatigue-driven cracking in concrete enhances chloride ingress and promotes further corrosion. These mutually reinforcing mechanisms lead to nonlinear degradation and significant reductions in service life, which cannot be captured by conventional sequential corrosion-fatigue analyses.
This contribution presents a fully coupled multiphysics phase-field modeling framework for corrosion-fatigue interaction in reinforced concrete. The framework consistently resolves the co-evolution of key physical processes, including chloride transport in concrete, corrosion initiation and reactive transport of iron species, rust precipitation and pressure buildup at the steel-concrete interface, corrosion-induced degradation of steel, fatigue damage in reinforcement, fracture and fatigue crack propagation in concrete, and damage-dependent transport properties. By embedding these processes within a unified chemo-mechanical formulation, the model explicitly captures feedback mechanisms between chemical degradation and mechanical damage.
The framework is implemented in FEniCS [https://doi.org/10.25835/3duuzvj4] and demonstrated through two-dimensional representative rebar configurations and a three-dimensional reinforced concrete beam. Numerical results reveal how corrosion state, loading history, and cyclic loading sequence govern crack initiation, corrosion kinetics, and fatigue lifetime. The simulations show that conventional corrosion-followed-by-fatigue approaches systematically underestimate structural performance, while the fully coupled model provides physics-based predictions of degradation and lifetime.
The proposed framework offers new insights into the spatio-temporal interaction between transport, cracking, and corrosion and represents a robust foundation for advanced lifetime assessment and future digital twin applications.

### A phase-field framework for rate-dependent failure in polymer fiber-reinforced high-performance concrete

Margalho de Barros, Marcos Andre; Brands, Dominik; Schröder, Jörg 08:50
*University Duisburg-Essen, Germany*

High-performance concrete (HPC) is characterized by its improved strength and durability when compared to “normal” concrete. However, it still exhibits brittle failure, prompting the use of fiber reinforcement to enhance their post-cracking performance. Steel fibers are commonly used for this purpose, but their susceptibility to corrosion in harsh environments, high density, and elevated energy footprint can render them less suitable. In contrast, polymer fibers offer a more sustainable alternative, being corrosion-resistant and significantly less dense than steel. Nevertheless, the intrinsically viscoelastic mechanical response of polymer fibers, the influence of environmental agents and loading magnitude and their impact on the failure of fiber-reinforced concrete remain insufficiently understood.

In this study, the phenomenological phase-field model introduced in [1]-[2] and later extended in [3] to include a transversely isotropic nonlinear viscoelastic formulation based on the Schapery model [4], is further developed to analyze the influence of different fiber orientations and volume fractions on the structural response of polymer fiber-reinforced HPC. In order to capture the failure in tension and compression of HPC, the step-wise linear degradation functions are used as introduced in [5]. Various orientation distribution functions (ODFs), accommodating different fiber orientations and statistical distributions, are implemented following [1]. Then, the three-point bending boundary value problem based on the EN14651 is carried out under different loading rates. Finally, the performance of the resulting numerical model is then evaluated using Load-CMOD (crack mouth opening displacement) curves.

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**Efficient Simulation of Fiber-Reinforced Concrete Considering the Micro-Mechanical Behavior of the Fiber-Concrete Interface**

Poriete, Paula; Curoșu, Verena; Löhnert, Stefan 09:10
*Institute of Mechanics and Shell Structures, TU Dresden, Germany*

Simulation of fiber-reinforced concrete on a composite scale is computationally challenging, as the slenderness of fibers necessitates the use of extremely fine meshes for the discretisation of the fiber material and the bulk material in the vicinity of each fiber, if largely skewed elements are to be avoided. Especially in three-dimensional simulations, the fine meshes lead to a significant increase in runtime. This contribution presents a remedy to the described issue, in which the explicit meshing of fiber geometry is circumvented by representing the fibers as one-dimensional manifolds embedded in the three-dimensional bulk material.
The one-dimensional fibers are coupled to the bulk material by a newly implemented connection element that contributes to the total energy potential in the form of an additional term that corresponds to the connection energy. The connection element formulation includes distinct constitutive
laws for the fiber-concrete interface in the directions normal and tangential to the fiber orientation. In the normal direction, relative displacements are constrained by means of the penalty
method, while in the direction tangential to the fiber orientation, the interface behavior is governed by a modified piecewise-linear traction-separation law that accounts for post-failure friction at the interface. For the automated and efficient generation of finite element meshes, an algorithm has been developed that can scatter one-dimensional fibers within the three-dimensional domain in a desired way, for example, with a bias towards a certain preferred fiber orientation, which could occur in practice during the manufacturing process of fiber-reinforced concrete.
The connection element formulation was firstly implemented in the initial configuration, but has been subsequently extended to the current configuration in order to allow the modeling of a large

fiber slip. The initial configuration integration scheme involves an integration point redefinition algorithm that preserves the properties of the applied quadrature rule in each connection element independently of the discretisation. The current configuration integration scheme considers small deformations for the fiber and the concrete materials, but allows for large fiber movements within the concrete material.
The application prospects of the implemented connection element involve not only the simulation of fully embedded fibers, but also the simulation of fiber pull-out from the bulk material, which is demonstrated by showcasing an emulated crack in the concrete matrix.

**Optimization maze solving algorithm for 3D-PRCSM multi-scale model analysis through ESDA**

Diaz, Guillermo
*Germany*

09:30

This work introduces a Global Crack Tracking Algorithm (GCTA) for the simulation of fracture in three-dimensional prestressed concrete structural members (3D-PRCSM), formulated within an energy-based, multiscale computational framework. The approach combines the Embedded Strong Discontinuity Approach (ESDA) with advanced constitutive models—anisotropic damage and generalized crystal plasticity—applied at the scale of each micro-component (cement paste, aggregates, reinforcing steel, and prestressing tendons). Instead of relying on classical homogenization schemes, the formulation directly composes the energetic and stress contributions of all constituent materials, enabling an accurate representation of local degradation, plastic flow, and interfacial debonding under highly heterogeneous stress states.

The core contribution of this research is the reinterpretation of crack propagation as an optimal path problem on a directed graph, solved using a maze-solving algorithm inspired by Dijkstra's method. Each Gauss point of the finite element mesh is represented as a node within a fracture-graph, whose edges encode a cost defined by the composite energy $\psi$c scaled by geometric distance. When the local fracture function becomes singular at a given integration point, the algorithm assigns a topological barrier ($\varphi$= –1), preventing further propagation through that node. This mechanism forces the system to identify minimum-energy crack paths, ensuring that the resulting fracture surfaces remain continuous, smooth, and physically meaningful, while avoiding remeshing, artificial regularization, or other non-physical smoothing techniques.

The proposed framework captures the simultaneous development of micro-cracking (within aggregates, rebars, and prestressing tendons) and macro-cracking at the structural level, while strictly enforcing the kinematic requirements of ESDA in three dimensions. Because the fracture-graph is fully constructed during preprocessing, the method operates efficiently on a fixed mesh and remains fully compatible with existing finite element codes.

Preliminary numerical investigations indicate that the GCTA improves the stability, convergence behavior, and physical reliability of 3D crack-path predictions in prestressed concrete under complex multiaxial loading. The algorithm successfully reproduces crack continuity across composite finite elements, resolves branching indirectly through energy-based detours, and enhances the robustness of post-peak simulations. Altogether, the proposed strategy constitutes a step toward a unified, energy-consistent, multiscale framework for the predictive analysis of failure mechanisms in 3D-PRCSM.

**Incorporation of fiber orientation state measures in the model-based design of fiber-reinforced concrete structures**

Neu, Gerrit Emanuel
*Ruhr University Bochum, Germany*

09:50

With ever-rising environmental concerns, designing more sustainable concrete structures is vital. Changing the composition of the cement paste or the use of recycled material are straightforward but essential steps to reduce the environmental impact of the construction sector. Another approach is to improve the methods of designing structures so that less material is required. Fiber Reinforced Concrete (FRC) shows great potential for material savings, improved durability, and the creation of more slender structures. An inherent challenge in the design of FRC structures is to address the

scatter in strength depending on the type, content, orientation and distribution of the fibers used as reinforcement. Guidelines determine the post-cracking strength of an FRC mixture by experiments, mostly some sort of bending test. The scatter in strength and the difference in fibre orientation between these characterization tests and the to-be-designed structural member are addressed by the application of respective safety factors and often lead to conservative designs.

In this contribution, a model-based investigation is carried out to relate fiber orientation measures to the post-cracking strength of FRC and with that provide guidance for the engineering design of FRC structures. For this, a multi-level model for the analysis of FRC structures is used, which allows to assess the influence of a chosen fibre type, content, and orientation on the structural response. Based on the explicit fibre geometry, the interface conditions, the material properties and an assumed fibre orientation, the model can be used to determine an equivalent uniaxial traction-separation law. In order to evaluate the post-cracking response of FRC structures by Finite-Element (FE) analysis, a discrete crack approach using interface-elements, whose post-cracking behavior is governed by the derived traction-separation law, is used. After providing an overview of experimental measures to describe the fiber orientation state, the model is validated by the re-analysis of experimental investigations, where the fiber orientation state is taken as explicit model input. A practical fiber orientation measure (e.g. orientation number) should be compared to a complete description of the fibre orientation state (based on CT scans) and the influence the fiber distribution and assumptions regarding the orientation state should be addressed. Finally, a parametric study is carried out to show the effect of different fiber orientation states on the structural performance of FRC members and provide guidance to link the post-cracking strength determined by bending tests to potential to-be-designed structural members.

**Mesoscale Modeling of Cohesive-Frictional Fracture Processes in Fiber-Reinforced Concrete**

Gudžulić, Vladislav 10:10
*Ruhr University Bochum, Germany*

Concrete is one of the most commonly utilized building materials and has a significant environmental footprint due to its production process. Over the past decades, considerable progress has been made in developing high-performance and ultra-high-performance concretes (HPC/UHPC) and incorporating fiber reinforcements in structural concrete, resulting in improved strength and durability and opening the possibility of creating slenderer structures, leading to significant material savings. However, adequate models and design approaches must accompany these material improvements to fully realize the potential benefits, especially considering the effects of the long-term sustained loads.

This work focuses on modeling material behavior of high- and ultra-high-performance fiber-reinforced concrete (HPFRC/UHPFRC), and investigating damage processes and mechanisms occurring at small scales, which are not readily observable during loading tests. To this end, it presents a framework based on image-derived mesoscale models generated from X-ray computed tomography (CT) scans of laboratory-scale specimens [1]. These models incorporate realistic aggregate and pore distributions as well as steel fibers, enabling detailed simulations of crack initiation and propagation processes. Crack initiation and propagation are governed by cohesive-frictional interfaces with crack dilatancy, while fibers and their coupling to concrete are represented explicitly using Timoshenko beam elements and a nonlinear bond-slip relation. This enables resolving the competition between frictional crack sliding, fiber pull-out, and matrix cracking at the mesoscale.

The proposed computational approach is validated against a number of experimental benchmarks, including uniaxial tension and compression experiments [1], three-point [2] and four-point bending tests [3], in which both the measured load-displacement responses and the experimentally observed transition from diffuse cracking to localized fracture are well captured.

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## S03.02: Multifuntional and Coupled

Date: March 17, 2026 16:30–18:30
Room: KII, M17.74
Chair(s): Kiefer, Björn
Ricoeur, Andreas

### Phase-field modeling of hydrogen-promoted ductile-to-brittle transition fracture: A chemical potential-based approach

Diddige, Vikas; Roth, Stephan; Kiefer, Bjoern 16:30
*Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany*

Green hydrogen is expected to play a major role in decarbonizing energy-intensive industries, but the rapid expansion of hydrogen production, storage, and transport infrastructure introduces serious integrity challenges. Structural alloys used across the hydrogen supply chain are susceptible to hydrogen embrittlement (HE), a degradation mechanism in which absorbed hydrogen reduces ductility, alters mechanical response, and can trigger premature failure under service loading. Although these alloys are normally highly ductile and fatigue resistant, hydrogen exposure can induce a transition from ductile to brittle fracture. Ensuring reliability therefore requires predictive tools capable of capturing both ductile and brittle crack propagation. Because experimental testing under realistic hydrogen conditions is costly and often impractical, robust numerical modeling frameworks are essential for material selection, component design, and structural integrity assessment.

Conventional numerical models for HE adopt hydrogen concentration as the primary field variable, with diffusion driven by concentration and hydrostatic stress gradients. This approach typically requires stress-dependent concentration boundary conditions to obtain physically consistent surface profiles under hydrogen exposure [1], as well as stress extrapolation or $C^1$-continuous finite elements. To overcome these numerical demands, a phase-field fracture model coupled to chemo-mechanics is formulated within a rate-variational framework [2], introducing chemical potential—the energy density conjugate to concentration—as an independent primary field variable [3,4]. This formulation naturally incorporates hydrostatic stress effects and eliminates ad hoc Dirichlet boundary conditions. Furthermore, since hydrogen reduces ductility and promotes a ductile-to-brittle transition, the classical brittle phase-field model is extended with plasticity to represent fracture and transition behavior within a Hydrogen-Enhanced DEcohesion (HEDE) mechanism.

The chemical potential–based formulation reproduces standard concentration-based lattice hydrogen profiles for specimens with uniform initial hydrogen and impermeable boundaries. Under environmental hydrogen charging imposed via Dirichlet boundary conditions, it predicts the expected subsurface concentration profile, whereas the conventional concentration-based model does not. As a result, the approach yields physically consistent load-to-fracture responses. The model also qualitatively captures the onset of sub-critical crack growth under sustained mechanical loading, reflecting the influence of evolving subsurface hydrogen. With plasticity included, the framework further predicts the HEDE-driven ductile-to-brittle transition, demonstrating its suitability for studying hydrogen-assisted fracture in ductile metals.

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**A Monolithic Scheme Coupling Chemo-Mechanics and the Non-Local Gurson-Tvergaard-Needleman Model for Hydrogen-Enhanced Ductile Damage**

Patil, Siddhi Avinash; Prüger, Stefan; Roth, Stephan; Kiefer, Bjoern 17:10
*TU Bergakademie Freiberg, Germany*

As various sectors transition from fossil fuels to hydrogen as a sustainable energy source, addressing hydrogen embrittlement in the safety assessment of steel components used for hydrogen production, transport, and storage becomes critically important. When these components are exposed to a hydrogen atmosphere, hydrogen readily diffuses into the metal lattice due to its small size and induces a ductile-to-brittle transition [1]. Ductile damage in steel is characterized by the nucleation, growth, and coalescence of microvoids—a process that is further accelerated in the presence of hydrogen.

The present work focuses on theories such as hydrogen-enhanced localized plasticity (HELP) and hydrogen-enhanced strain-induced vacancies (HESIV), which accelerate the ductile damage [2]. To address this, we propose a mesh-independent finite element framework by combining coupled chemo-mechanics and the non-local Gurson-Tvergaard-Needleman (GTN) damage model [3]. This fully-coupled framework is motivated by Fick's law for standard diffusion and the mixed rate-type potential approach introduced in [4], which accounts for the influence of hydrogen concentration on the material's mechanical response. Moreover, the effects of hydrogen on damage are incorporated by extending the original non-local GTN model to account for hydrogen-enhanced void growth and nucleation, as suggested in [1, 2]. The stress-diffusion coupled system of equations is solved using a monolithic approach. In contrast to our previous work [1], based on a staggered scheme formulated within a small deformation setting, the present monolithic framework is implemented in a finite deformation setting, ensuring more realistic damage predictions. Furthermore, it exhibits improved convergence compared to the traditional sequential approach, with enhanced robustness in handling the choice of material parameter values. The mutual interactions are explored in various representative boundary value problems to assess the impact of hydrogen on material degradation and the stress state on diffusion.

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**A New Take on Sharp Cracks in Brittle Dielectrics: Where Electric Dipole Layers Meet Concentrated Line Forces**

Behlen, Lennart (1); Wallenta, Daniel (2); Ricoeur, Andreas (1) 17:30
*1: University of Kassel, Institute of Mechanics, Germany*
*2: University of Kassel, Institute of Mathematics, Germany*

Multifunctional or so-called smart materials take a special role in technical applications, as they are oftentimes not only subjected to mechanical loading, but also electric or magnetic fields for purposes such as actuating or controlling. To this end, dielectric and piezoelectric ceramics have been investigated in depth over the last decades, where the latter even possess a desirable electromechanical coupling on the constitutive level. These materials, expected to endure millions of loading cycles in long-term applications such as energy harvesting, are prone to brittle fracture originating in sharp

cracks, which are commonly analyzed within the theory of linear-piezoelectric fracture mechanics. Prior to recent developments, this theory mainly focused exclusively on mechanical tractions at the boundary of the body as well as electrostatic surface forces at the crack faces, which generally effectuate a crack closing.

In this work, the integral formulation of the electrostatic force acting on cracked isotropic dielectrics according to different established models of the Maxwell stress tensor is carefully investigated. As a consequence, additional volume forces may emerge in the interior of the body, which are shown to result in a higher-order stress singularity at the crack front. Beyond that, by rigorously following the Maxwell stress theory, it is revealed that unnoticed concentrated line forces act upon the fronts of semi- or impermeable cracks. At first glance, a physical interpretation of these line forces seems difficult. Exacerbating the issue, an apparent paradox occurs with respect to the so-called Lorentz model when recalling that there exist neither free nor bound charges in the vicinity of the crack front. The resolution of this situation involves a revisit of the concept of electric dipole layers from the theory of electrostatics, which are known to result in a jump of electrostatic potential along the surface they are distributed on. Finally, the occurrence of line forces acquires physical justification and a striking parallel between conducting and impermeable cracks is drawn.

**Crack Propagation in Superelastic Shape Memory Alloy-Based Elastocaloric Materials**

Grupp, Tim (1); Louia, Franziska (1); Motzki, Paul (1,2) 17:50

*1: Saarland University, Department of Systems Engineering, Germany*
*2: Center for Mechatronics and Automation Technology (ZeMA gGmbH), Germany*

The increasing global demand for efficient and sustainable cooling technologies has brought elastocaloric systems, which utilize the latent heat exchange of Shape Memory Alloys (SMAs), into focus as the most promising alternative to conventional vapor compression refrigeration. As an emerging and innovative technology, elastocaloric cooling shows exceptional promise due to its high coefficient of performance, use of solid-state refrigerants, and zero global warming potential. However, the commercialization of tension-based systems is critically limited by the fatigue life of the SMA elements under cyclic mechanical loading. To address this challenge, this contribution investigates the fatigue behavior, material lifetime and failure mechanisms associated with NiTi SMAs used in elastocaloric applications.

The thermo-mechanically coupled transformation behavior of superelastic SMAs is modeled using the one-dimensional Müller-Achenbach-Seelecke constitutive model [1,2], grounded in statistical thermodynamics. The influence of localized phase transformation effects [3] on crack propagation is analyzed within a phase-field framework. The theoretical framework is implemented into the finite element software COMSOL Multiphysics to explore the influence of temperature, transformation stresses and stress-strain hysteresis. These findings support early detection of fatigue damage, enhancing the reliability and performance of elastocaloric cooling systems.

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**S03.03: Ice / Snow / Hydraulic Fracture**

Date: March 18, 2026 14:00–16:00
Room: KII, M17.74
Chair(s): Weißgraeber, Philipp

**A model for mode partitioning: Identifying the mixed-mode fracture toughness for weak snow layers**

Rheinschmidt, Florian (1); Adam, Valentin (2); Rosendahl, Philipp L. (2); Weißgraeber, Philipp (1) 14:00

*1: Chair of Lightweight Design, University of Rostock, Germany*
*2: Institute of Structural Mechanics and Design, Technical University of Darmstadt, Germany*

In recent years, test campaigns were conducted to identify the interaction between fracture modes I- and II for weak snow layers [1]. The interest for these properties arises from the role, that the fracture toughness plays in governing anticrack propagation. This propagation is an important step that links the local failure of the snow slab with dry-snow slab avalanche release.

However, in three-dimensional numerical studies, the propagation behavior of the anticrack in the weak layer is also dependent on the direction of crack advance [2]. While anticrack propagation in the downslope direction is governed by an interaction between fracture modes I- and II, for cross-slope propagation mode III can no longer be excluded.

Measuring the mode III fracture toughness is challenging, especially under field conditions where no laboratory equipment is available. The present study develops of a novel test setup, which employs a portable motor unit to conduct displacement-controlled tests on site. The basis for our test is the ODCB test which enables researchers to investigate the mixed I/III mode fracture toughness [3].

The displacement-controlled setup is a crucial improvement for field tests and enables us to reduce the scatter that is observed in other field experiments. To derive the critical energy release rates, a novel closed-form model based on calculus of variations is employed. The model can render stress distributions in the weak interface in real time. Additionally, the full displacement field of the overlying snow slab is rendered by including FSDT and torsion [4]. To compute the energy release rate of anticracks in the weak interface, an adapted J-integral is employed. It includes the effect of the gravitational loading and can identify the energy release rate within one computation. Moreover, the obtained expression allows for a mode partitioning into the three fracture modes I, II and III. With this, the experimental results can be evaluated to identify the mixed-mode fracture toughness between all three modes.

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**Fracture and calving front evolution: A case study of Fimbul Ice Shelf, Antarctica**

Humbert, Angelika (1); Höyns, Lea-Sophie (1); Skatulla, Sebastian (2); Shoko, Moreblessings (2); Odera, Patroba (2); Yumbu, Alex (2); Dookee, Bhooshay (2); Floricioiu, Dana (3); Müller, Ralf (4); Sondershaus, Rabea (4) 14:20

*1: Alfred-Wegener-Institut Helmholtz Zentrum für Polar- und Meeresforschung, Germany*
*2: University of Cape Town, South Africa*
*3: German Aerospace Center, DLR, Germany*
*4: TU Darmstadt, Germany*

Ice shelves are fringing the Antarctic ice sheet, and their buttressing is stabilising outlet glaciers and ice streams. Natural calving of tabular icebergs is initiated by episodic fracture evolution, as glacier ice behaves as a brittle viscoelastic material in the typical load situations in glaciers. The position of the calving front, the lateral margin of ice shelves, is strongly influenced by the presence of ice rises, which are areas where the floating ice shelves are grounded. Ice rises lead to shear and tensile stresses in their vicinity, which promote crack formation and propagation. In this presentation, we focus on Fimbulisen, an ice shelf fringing Dronning Maud Land, with the characteristic Trolltunga,

that broke off as a giant iceberg in 1967 and has been regrowing since then. We use optical and radar satellite imagery to detect fractures and observe their evolution since the 1980s. High-resolution radar imagery enables us to detect crack tip patterns, from which we can reconstruct the episodes of fracture propagation. We compare this to simulated stresses using inverse modelling based on the higher-order stress balance of Fimbulisen. Furthermore, we present an example of fracture phase field modelling for ice rises at calving fronts.

**On the influence of spin up simulations on fracture in ice shelves**

Sondershaus, Rabea (1); Humbert, Angelika (2,3); Müller, Ralf (1) 14:40

*1: Technische Universität Darmstadt, Germany*
*2: Alfred-Wegener-Institut Helmholtz Zentrum für Polar- und Meeresforschung, Germany*
*3: University of Bremen, Germany*

Calving describes the process of iceberg break-off from the Antarctic and Greenlandic ice sheets. Since ice shelves stabilize inland glaciers, calving has a strong influence on both glacier dynamics and ice sheet stability. Glacier ice can be described as a Maxwell-type material, responding elastically on short and viscously on long time scales to loading. The mechanical response of viscoelastic materials is governed not only by the current deformation but also by the entire history of previously applied deformations. At the calving front, the lateral margin of glaciers and ice shelves, the ice cannot be considered as unloaded instead it has undergone prolonged deformation. This study investigates how such deformation history influences fracture processes at the calving front to better understand calving. For this purpose spin up simulations of a Greenlandic ice shelf are conducted in three-dimensions at finite strains, where the ice shelf is modeled over different time periods, to generate distinct initial states and history fields for fracture. With the different initial states fracture simulations are carried out, where fracture in the domain is modeled by means of a viscoelastic phase field model. The influence of the spin up duration on the crack evolution is analyzed.

**Fracture Phase-Field Modeling of Supraglacial Lake Drainage and Marine Ice Cliff Instability**

Benkert, Svenja (1); Hanfland, Celina (2); Hessenthaler, Lisa (3); Krahl, Jonathan (4); Riedel, Marit (5); Schmidt, Konstantin (6); Steppe, Johannes (7); Teschner, Phillip (1) 15:00

*1: University of Göttingen*
*2: Paderborn University*
*3: Karlsruhe Institute of Technology*
*4: ETH Zürich*
*5: Heidelberg University*
*6: TU Munich*
*7: University of Freiburg*

Sea level rise is strongly influenced by mass loss from the Greenland and Antarctic ice sheets, which is the imbalance of accumulation of snow over the ice sheet and the discharge of ice across the grounding line. Fundamental mechanical processes such as crack formation are playing a key role in glacier dynamics, e.g. calving and instability of ice cliffs and the formation of crevasses leading to drainage of supraglacial lakes.

Several mechanisms have been discussed to enhance mass loss. One proposed process is the Marine Ice Cliff Instability (MICI), relevant in Antarctica where tall marine-terminating ice cliffs occur. MICI describes the yet unobserved self-sustaining collapse of exposed high ice cliffs after the disintegration of the ice shelf, which can speed up glacier flow and trigger positive feedback, particularly on retrograde beds.

Another important mechanism is the flooding of the subglacial hydrological system, particularly regarding the drainage of supraglacial lakes through cracks. Since observations suggest that drainage locally accelerates the glacier flow, it is hypothesized that large inputs of meltwater into the drainage system lubricate the glacier base and increase overall flow speeds.

To model these two phenomena, we employ a fracture phase field method, which is based on the variational theory by Griffith. The degradation state of the material is represented by a continuous scalar field. Therefore, the crack is not a sharp contour but smeared out. This framework enables modeling of crack initiation and propagation without explicitly tracking crack faces and costly re-meshing.

Glacial ice is a viscoelastic material. However, we assume linear elasticity, as crack initiation and propagation occur on short time-scales on which the viscous behavior is negligible.
In this contribution, we study crack formation and propagation on a two-dimensional flow-line cross section of a glacier for both MICI and lake drainage scenarios. For the former, we examine the impact of different cliff heights (freeboards), while for the latter, we focus on the roles of water and initial hairline cracks. In both cases, we analyze crack depths and positions.

**On the Computation of Crack Surface Normals in the Framework of the Phase-Field Model of Hydraulic Fracturing**

Gupte, Anuj; Polukhov, Elten; Keip, Marc-André
*University of Stuttgart, Germany*

15:20

Hydraulic fracturing techniques have been used to extract oil from the Earth's crust and to enhance the efficiency of geothermal systems among other applications. Numerical simulation of hydraulic fracturing is essential for predicting the environmental impact of this method, as well as its efficiency in such applications. In the present work, our aim is to investigate fluid-driven fracturing in porous materials by employing a phase-field model of fracture within Biot's poroelasticity theory [1, 2].

In this context, a major challenge in the simulation of hydraulic fracturing is the accurate computation of the normals to the regularized crack surface. This challenge arises due to vanishing gradients of the phase-field variable in fractured zones. To overcome this issue, several methods have been proposed to compute the normal of the crack surface. For instance, the $L_2$-projection of the phase-field gradients is exploited in [3] to determine the crack normals in entirely fractured finite elements. Another approach, proposed by [4], identifies the crack normals as the principal directions of the strain tensor corresponding to its largest principal value. In the present contribution, we explore these approaches and show that, in certain scenarios, they yield spurious normals at the crack tip or at the fluid-mass injection boundary. Our investigations are carried out within finite-element implementations using Lagrangian interpolations of first- and second-order elements ($Q_4$ and $Q_9$), as well as divergence-conforming Brezzi-Douglas-Fortin-Marini finite elements of second-order ($BDFM_2$) [5]. We further provide an alternative approach to improve the accurate computation of the normals at the crack surface.

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**Crack Surface Normal Computation via Clustering and Ridge Regression to Model Hydraulic Fracture**

Marulkar, Vedant Satish; Polukhov, Elten; Keip, Marc-André
*University of Stuttgart, Germany*

15:40

Hydraulic fracture plays a crucial role in energy and environmental applications, including oil and gas recovery and geothermal energy extraction. Accurate hydraulic fracture modeling requires resolving fluid flow in both the porous medium and evolving cracks, which are described by Darcy flow and

Poiseuille flow within the framework of Biot's theory, respectively [1]. A central challenge in the phase-field modeling of hydraulic fracture is the accurate determination of crack surface normals. These normals are used for the computation of crack opening in Poiseuille-type flow and, consequently, for defining the anisotropic permeability tensor. Direct evaluation of normals using phase-field gradients often produces unreliable results in fully fractured zones and near crack tips [2]. Moreover, $L^2$-projection techniques may fail to produce meaningful normals in regions with high curvature or branching. The objective of the present contribution is to develop a robust dynamic algorithm to compute meaningful normals for arbitrary fracture geometries by reconstructing crack paths, following the recently proposed approach of [3].

In our approach, after each time step, nodes exceeding a prescribed phase-field threshold are clustered using a two-dimensional k-means algorithm to account for multiple cracks. Within each cluster, the crack path is fitted as a smooth curve using ridge regression. Normals along the fitted path are computed using a central finite-difference scheme and are subsequently projected back onto the original fractured nodes. The algorithm seamlessly integrates with hydraulic fracture simulations [4]. Incorporating this approach for computing crack surface normals in hydraulic fracture modeling improves accuracy and stability. In the presentation, in addition to the algorithmic implementation, we discuss various test cases used for validation of the proposed approach.

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## S03.04: Fatigue

Date: March 18, 2026 16:30–18:30
Room: KII, M17.74
Chair(s): Tsakmakis, Aris

### Modelling of fatigue crack propagation in ductile materials under non-proportional loading conditions

Tsakmakis, Aris; Gibb, Alwin 16:30
*Materials Mechanics Group, Technical University of Darmstadt, Germany*

The aim of this research is to simulate fatigue crack propagation in ductile materials subjected to proportional and non-proportional, cyclic loading conditions. For the materials under consideration, it is expected that non-proportional hardening has a major influence on the crack initiation and further evolution.
Consequently, the first part of this work focuses on the modeling of the constitutive response for non-proportional cyclic loading conditions. The hardening mechanisms considered here are isotropic and kinematic hardening in conjunction with a deformation-induced, formative and a rotational change of the yield surface. The latter is captured by introducing a fourth-order tensor into the von Mises yield condition. A first attempt to model such a material behavior was presented in Dafalias et al. [1]. In the second part of this work, the constitutive equations are extended by a further internal variable, the phase field (or damage) variable, to describe ductile crack growth, cf. Tsakmakis and Vormwald [2]. It is assumed, that the underlying crack growth mechanism is driven by plastic deformation. Consequently, a damage evolution equation from classical continuum damage mechanics is adapted. The model features furthermore an additional term in the plastic part of the free energy density which is introduced for modelling the material response under fatigue loading. Both parts of the proposed

model are formulated thermodynamically consistent and corresponding material parameters are calibrated experimentally.
Finally, the capabilities of the proposed model are analyzed with the help of experimental results. Numerically predicted and experimentally determined crack paths in thin-walled tubes under combined tension/compression and torsional, cyclic loading are compared. In particular, both, proportional and non-proportional loading conditions are investigated.
In order to accelerate the fatigue simulations and reduce the (very high) computational cost that arises, a cycle skipping technique is implemented. The comparison of experimental and numerical results shows that, for proportional loading conditions, there is only a quantitative influence of the hardening with respect to the crack growth rate. For non-proportional loading, however, there is a significant influence on the hardening mechanisms concerning the predicted crack paths. This highlights the necessity for accurate modelling of the deformation behavior in such loading cases.

**Phase field modeling of thermal fatigue in ductile materials**

Gao, Hanghang; Ma, Songyun; Markert, Bernd 17:10
*Chair and Institute of General Mechanics, RWTH Aachen University, Germany*

Fatigue damage is one of the most common failure mechanisms in industrial structures, often leading to catastrophic failures of mechanical components or systems in airplanes, automobiles, trains, etc. Due to the requirement of aerodynamic, thermal, and mechanical performance, engineering components are commonly complex in shape and subjected to multiaxial thermo-mechanical loading conditions. Thermo-mechanical fatigue is a complex failure mechanism resulting from thermal and mechanical stresses. The interaction of these stresses significantly influences the evolution of material microstructure, leading to coupled effects involving creep, fatigue, and environmental degradation. Understanding and accurately predicting thermo-mechanically coupled fatigue behavior of metallic materials are crucial for ensuring the structural integrity and operational reliability of mechanical components under high-temperature service conditions.

In the present work, a thermodynamically consistent phase field fatigue model is extended to describe the thermal fatigue behavior of elasto-viscoplastic materials under cyclic thermo-mechanical loadings. The proposed model is developed based on a variational framework. An additional energy accumulation variable is introduced to capture the progressive accumulation of fatigue damage over loading cycles. Furthermore, a cyclic viscoplasticity model is employed to account for the nonlinear inelastic deformation behavior during the fatigue process. Several numerical examples are presented to demonstrate the model's predictive ability of the thermo-mechanical fatigue behavior.

**Advances in High-Cycle-Fatigue Modeling – Utilizing the Endurance Surface Continuum Damage Model**

Feike, Klas; Kurzeja, Patrick; Mosler, Jörn 17:30
*TU Dortmund University, Germany*

Cyclic loading occurs in numerous engineering applications, ranging from classic tubular shafts in drivetrains to the wings and fuselage of aircraft. Understanding and accurately predicting fatigue behavior under such conditions is therefore essential. This work aims to model the fatigue response of metals in the high-cycle fatigue regime – not only under controlled laboratory conditions but also for service scenarios involving complex load paths.

In this regime, material degradation typically exhibits quasi-brittle characteristics from a macroscopic viewpoint. Damage is primarily driven by the elastic energy [1]. To capture this behavior, a continuum damage framework inspired by the endurance surface concept is integrated into an established model based on the effective configuration concept [2-4]. The formulation ensures thermodynamic consistency and incorporates spatial gradients of the damage field through a micromorphic enhancement, yielding physically meaningful and mesh-independent results [5-6].

The performance of the proposed model is first shown for monotonic loading by the example of concrete. It is then extended to cyclic loading conditions by the example of low-alloy steel. Benchmark simulations demonstrate its predictive capabilities across various loading scenarios. A particular emphasis is on non-proportional load paths. This challenging setting can arise from uncertain or changing load conditions in practical applications. Accordingly, the framework's ability to represent anisotropic damage evolution is of high practical interest and is demonstrated in terms of versatility for advanced fatigue modeling applications.

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**Microscopic crack propagation caused by high-cycle loading in reused reinforcing steels**

Miska, Niklas; Balzani, Daniel 17:50
*Ruhr-Universität Bochum, Germany*

The reuse of concrete elements, which are extracted from old buildings during demolishing, in new buildings is an emerging research topic and faces several yet unanswered challenges. One of such challenges is the assessment of durability of the utilized reinforcing steels, in particular in view of the variety of production processes used decades ago as well as the potential presence of initial microcracks due to construction, loading and deconstruction. In addition to that, the reinforcing steels will experience a significantly larger number of loading cycles due to the reuse in new buildings than the standards have accounted for at construction time. Thus, it is important to investigate the load-bearing capacity of such reused steels which reduces with high numbers of loading cycles. Since it is not feasible to test all reinforcing steels experimentally, the load-bearing capacity is assessed in terms of a virtual lab by means of numerical finite element simulations. In this contribution, the software package DAMASK is utilized to simulate the reinforcing steel on the microscale accounting for the polycrystaline structure. Even though DAMASK allows for the utilization of FFT-solvers and thus, a rather efficient simulation of polycrystals and crystalplasticity is enabled, the simulation of a large number of loading cycles, i.e. $10^6$, is still not realizable. Thus, we present the combination of the simulation in DAMASK with a cycle-jump approach, in which only a few cycles are computed by finite elements and the majority of cycles is approximated by time-integration schemes for the evolution of the internal variables. By that, a more efficient assessment of the remaining load-bearing capacity of the reinforcing steel microstructure is enabled.

**Phase-field modeling of time-dependent fatigue in hydrogels**

Wei, Yujie; Ma, Songyun; Markert, Bernd 18:10
*RWTH aachen University, Germany*

Hydrogels are soft materials composed of water and crosslinked polymer networks. They exhibit excellent biocompatibility and flexibility, rendering them widely applicable in drug delivery, soft robotics, and 3D printed tissues. In many of these applications, hydrogels are subjected to cyclic loadings, leading to progressive fatigue damage and eventual failure. Therefore, predicting the fatigue behavior of hydrogels is important for ensuring the long-term chemomechanical performance. However, computational fatigue assessment methods specifically developed for hydrogels are not well established.

Most existing fatigue models treat hydrogels as pure solids under finite strain assumptions, neglecting the critical role of fluid flow within the polymer network. Moreover, the time-dependent effects of fluid migration and polymer-network relaxation on the fatigue behavior are still insufficiently studied .

To address these limitations, this study proposes a phase-field approach to predict the fatigue process in hydrogels. A viscoelastic model is employed to describe the time-dependent large deformation behavior of the polymer skeleton. Additionally, Darcy's law is used to characterize the fluid transport in hydrogels. The proposed model captures the time-dependent fatigue behavior induced by both viscoelastic deformation of polymer network and pore pressure-driven fluid flow, providing an effective approach for predicting fatigue in hydrogels.

## S03.05: Dynamic Fracture / Peridynamics

Date: March 19, 2026 08:30–10:30
Room: KII, M17.74
Chair(s): Wieners, Christian

### A Dynamic Phase-Field Framework with Automatic Mesh Adaptivity for Fast and Stable Fracture Simulation

Saberi, Hossein; Düster, Alexander 08:30
*Technische Universität Hamburg (TUHH), Germany*

This study presents an efficient adaptive phase-field framework for simulating dynamic brittle fracture with the material damping effects. A mesh refinement strategy is developed based on a node-distance function driven by the evolving phase-field variable, enabling the mesh to automatically refine in regions of high damage without prior knowledge of the crack path. During the simulation, new field nodes are inserted when the local nodal spacing exceeds an adaptively defined threshold, allowing the mesh to evolve consistently with crack propagation while significantly reducing computational cost. A staggered solution strategy is proposed, in which displacement and phase-field variables are iteratively updated within each time step to maintain solution consistency. The proposed methodology is validated through three numerical examples, evaluating elastic strain energy, kinetic energy, and fracture energy, as well as the influence of material damping. The results confirm that the adaptive phase-field framework offers high accuracy, improved efficiency, and robust convergence performance in dynamic fracture simulations.

### Dynamic Phase Field Fracture Simulation Using a Spatio-Temporally Adaptive Asynchronous Variational Integrator

Jadhav, Deepak B. (1); Phansalkar, Dhananjay (2); Weinberg, Kerstin (3); Ortiz, Michael (4); Dornisch, Wolfgang (1); Leyendecker, Sigrid (2,5) 08:50
*1: Lehrstuhl für Technische Mechanik (LTM), RPTU Kaiserslautern, Germany*
*2: Lehrstuhl für Technische Dynamik (LTD), FAU Erlangen, Germany*
*3: Lehrstuhl für Festkörpermechanik, Universität Siegen, Germany*
*4: Division of Engineering and Applied Sciences, California Institute of Technology, USA*
*5: Faculty of Engineering, School of Mechanical, Medical & Process Engineering, Queensland University of Technology, Australia*

Phase field modeling of fracture has emerged as a fundamental and effective approach forsimulating crack propagation. The phase field model represents the discrete crack as a smearedcrack within a variational framework. This approach eliminates the need for explicit cracktracking algorithms and allows for effective modeling of complex fracture behaviors such askinking, branching, merging, and coalescence. Despite these advantages, the phase fieldformulation inherently involves a length scale parameter $\varepsilon$that governs the width of thesmeared crack zone. Without apriori knowledge of the direction of the crack propagation, thespatial mesh must be uniformly fine throughout the entire computational domain to accuratelyresolve $\varepsilon$. This requirement of a uniformly fine mesh leads to substantial computational costs,especially in dynamic fracture simulations, where the global time step is determined by thesmallest spatial element of the mesh.

To address this challenge, a recently proposed asynchronous variational integrator (AVI) forphase field modeling of dynamic fracture allows each spatial element in the mesh to advancein time using its own characteristic time step. In this framework, the mechanical fields areupdated at each elemental time step, while the phase field is updated only after the mechanicalupdate of the largest spatial mesh element [1,2]. We extend this AVI framework byincorporating phase field driven spatial mesh adaptivity. The computational domain isdynamically refined based on a given threshold value of the phase field and then the time stepsof the elements are also recalculated accordingly. This leads to a fully spatio-temporallyadaptive AVI formulation for dynamic fracture problems, where spatial adaptivity is driven bythe evolving fracture phase field, and temporal adaptivity is inherently provided by the AVI.Benchmark examples shows that the proposed approach achieves notable computationalsavings without compromising accuracy.

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[2] Jadhav D. B., Phasalkar D., Weinberg K., Ortiz M., Leyendecker S. A New Approach toAsynchronous Variational Integrators for a Phase Field Model of Dynamic Fracture.International Journal for Numerical Methods in Engineering 2025; 126(6) : e70025.

**From stationary to growing cracks: The Virtual Element Method in dynamic fracture mechanics**

Wappler, Philipp; Ricoeur, Andreas 09:10
*University of Kassel, Germany*

A critical look at existing numerical approaches for the analysis of dynamically loaded cracks in brittle materials reveals persistent challenges in the field of dynamic fracture mechanics. The precise resolution of fracture mechanics quantities, the consistent calculation of crack tip velocities, the consideration of material damping, and constantly changing mesh topologies remain demanding tasks. To overcome these challenges, standard finite element techniques require inefficient remeshing and mesh mapping procedures, while enrichment methods involve complex subroutines for integration and postprocessing. Frequently used phase field models necessitate a comparatively fine discretization for crack propagation and are sensitive to mesh parameters. The Virtual Element Method (VEM), presented in 2013 by Beirão Da Veiga et al. [1], is a modern stabilized Bubnov-Galerkin method and has been identified as a promising candidate for more efficient solutions in works, e.g., by Choi et al. [2] or Chen et al. [3]. Key advantages result from the outstanding mesh flexibility, which allows the straightforward integration of crack tips into element geometries, as well as specific refinement techniques for fracture mechanics applications, such as cohesive zone models. Despite its promising properties, VEM is rarely used for discrete modeling of cracks in the context of dynamic calculations.

The presentation demonstrates the VEM for dynamic crack tip loading analyses of stationary cracks in the time and frequency domains, especially for impact and cyclic external loads. The results are, if available, validated against analytical solutions and benchmarks from the literature. Eventually, established numerical approaches of dynamic crack growth simulations are critically discussed.

**References**

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[2] H. Choi, H. Chi, and K. Park, “Virtual element method for mixed-mode cohesive fracture simulation with element split and domain integral,” *Int J Fract*, vol. 240, no. 1, pp. 51–70, Mar. 2023, DOI: 10.1007/s10704-022-00675-7.

[3] Y. Chen, D. Sun, U. Perego, and Q. Li, “Brittle crack propagation simulation based on the Virtual Element Method and $J_k$ -integral fracture criterion,” *Engineering Fracture Mechanics*, vol. 314, p. 110684, Feb. 2025, DOI: 10.1016/j.engfracmech.2024.110684.

**Estimating Forming-Induced Damage for Crash Simulations with LS-Dyna**

Zink, Thomas (1,2); Böhlke, Thomas (2); Burbulla, Frank (1); Bencker, Sebastian (1) 09:30
*1: Dr. Ing. h.c. F. Porsche AG, Weissach, Germany*
*2: Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Germany*

Accurate crash simulations require the consideration of manufacturing effects such as thinning, plastic strain and forming-induced damage. While thinning and strain mapping from forming to crash have become industrial standard, the transfer of damage is still unresolved. A direct hand-over of damage variables is typically not feasible, since forming and crash simulations rely on different solvers and material models. As a result, damage that occurs during the forming process is frequently estimated instead of being transferred directly.

In crash simulations with LS-Dyna, sheet metal parts are commonly discretized with shell elements under plane-stress assumptions. Plasticity is represented by a von Mises model with isotropic hardening, while damage and failure are described by the Generalized Incremental Stress State-Dependent Damage Model (GISSMO), where damage accumulation depends on plastic strain and stress triaxiality.

This work introduces a method to estimate forming-induced damage based on the relationship between plastic strain, through-thickness strain and stress triaxiality. The forming process is represented as a sequence of intervals with constant triaxiality. Exploiting the linear correlation between triaxiality and the ratio of plastic strain to through-thickness strain under plane-stress conditions enables computing damage estimates as well as upper and lower bounds of accumulated damage consistent with the observed strain and thinning after forming.

The method is evaluated using geometries ranging from a deep-drawn cup to an industrial door blank. Estimated damage values are compared to forming simulations with GISSMO, demonstrating a close agreement in the spatial distribution and magnitude of predicted damage. The proposed method provides a computationally efficient way to extend forming simulations to include damage and supports early assessment of forming-induced damage effects in subsequent crash analysis.

**Ghost Forces and Dual-Horizon Bond-Based Peridynamics: A Variational Mechanics Perspective**

Capobianco, Giuseppe; Prateek, Prateek; Leyendecker, Sigrid 09:50
*Institute of Applied Dynamics, FAU Erlangen-Nürnberg, Germany*

It is known that applying the dynamical equilibrium equations of bond-based peridynamics with variable horizon leads to 'ghost forces' that lead to spurious wave reflections. As a remedy, the dynamical equilibrium equations have been extended to include a dual horizon contribution that compensates the effect of ghost forces and led to the advent of dual horizon peridynamcs. In this talk, we will shed some light on 'ghost forces' and dual horizon bond-based peridynamcs form the viewpoint of variational mechanics. We will show that, for variable horizons, the internal forces of the dynamical equilibrium equations of bond-based peridynamics do not fulfill the principle of interaction, and hence act like external forces perceived as 'ghost forces'. Moreover, we will derive the dynamical equilibrium equations for bond-based peridynamics from Hamilton's principle of stationary action and show that this naturally leads to the dual horizon peridynamics formulation in the case of variable horizon.

**A novel adaptive approach to bond-associated peridynamics**

Partmann, Kai (1); Wieners, Christian (2); Weinberg, Kerstin (1) 10:10
*1: Chair of Solid Mechanics, University of Siegen, Siegen, Germany*
*2: Institute of Applied and Numerical Mathematics, KIT, Karlsruhe, Germany*

Peridynamics is a nonlocal continuum mechanics formulation that is particularly well-suited for simulating dynamic fracture in materials. The correspondence formulation addresses the limitations of earlier peridynamic formulations by enabling accurate elastic behavior and facilitating the use of

classical constitutive models. However, it suffers from stability issues due to zero-energy modes. Relations of the correspondence formulation to the Reproducing Kernel Particle Method, the Element-Free Galerkin method, and Smoothed Particle Hydrodynamics have been established in the literature. It can be shown that the instabilities are similar to those observed in other meshfree methods with nodal integration. Bond-associated peridynamics has been proposed as a stabilization technique that approximates the deformation gradient on a per-bond basis, similar to higher-order integration schemes in other meshfree methods. However, this approach increases computational costs.

This study presents an adaptive approach where bond-associated modeling is applied only in regions and time intervals where it is necessary. The proposed adaptive strategy reduces computational costs by applying the expensive scheme only where needed while using the unstabilized correspondence formulation elsewhere. Numerical experiments demonstrate that the adaptive criterion captures instabilities of the unstabilized correspondence model very well, making this approach a valid method for improving the stability of classical correspondence modeling. It is also demonstrated that the approach can be used to model dynamic fracture problems efficiently.

## S03.06: Heterogeneities / Contact / Friction

Date: March 19, 2026 14:00–16:00
Room: KII, M17.74
Chair(s): Ricoeur, Andreas

### Influence of Material Constitutive Laws on Effective Crack Resistance in Heterogeneous Materials

Schlüter, Alexander; Müller, Ralf 14:00
*Technische Universität Darmstadt, Institut für Mechanik, Kontinuumsmechanik, Germany*

This work focuses on studying how different material constitutive laws influence the effective crack resistance in heterogeneous materials. Building on the numerical framework of Hossain et al. [1], we perform simulations that allow the effective crack resistance to be identified as a material parameter. Displacement boundary conditions corresponding to a steadily advancing macroscopic crack are applied to a representative microstructure, while crack growth on the microscale is modeled without imposing assumptions on crack paths or propagation continuity using a phase-field model for fracture. The maximum value of the macroscopically evaluated J-integral provides the driving force required to extend the crack by a macroscopic increment without arrest and is used to define the effective crack resistance. The study places particular emphasis on how different material behaviors affect the predicted fracture resistance. Dissipative effects are examined through von Mises plasticity, while general nonlinear responses are characterized using a Ramberg–Osgood formulation.

[1] M. Z. Hossain, C. J. Hsueh, B. Bourdin, K. Bhattacharya, *Effective toughness of heterogeneous media*, Journal of the Mechanics and Physics of Solids 71, pp. 15–32.

### Prediction of Interface Crack Deflection in Bimaterials Using the J-Integral for Cohesive Zones

Zarjov, Konstantin; Ricoeur, Andreas 14:40
*Universität Kassel, Germany*

Composites represent a class of engineering materials can be tailored over a wide range by the addition of additives. However, improvements in specific target properties may also lead to reductions in strength. The optimal selection of additives therefore requires an understanding of damage processes in the microstructure at the length scale of the additives.

For understanding damage processes, the simulation of delamination and crack transitions is essential. Cohesive zone models are particularly well suited for simulating debonding processes; however, limitations arise when modeling crack transition from the interface into the adjacent material. To address this, a suitable deflection criterion has been developed. This criterion is based on a modified cohesive J-integral [1], which has so far been verified for straight interfaces in monomaterials.

The combination of additives and matrix forms a bimaterial system with mismatched elastic properties and fracture toughnesses. Depending on processing and the type of additives, interfaces exhibit a wide variety of shapes. As a result, delamination generally involves curved interface cracks.

Reliable quantification of crack-tip loading therefore requires a cohesive J-integral formulation that is applicable to bimaterials and curved cracks. The present work aims to verify these two aspects and to investigate the influence of elastic as well as fracture-mechanical discontinuities at the interface. Ultimately, the anisotropic crack deflection criterion based on the J-integral vector is to be qualified as a reliable tool for predicting crack growth during delamination processes at interfaces in composites.

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**Modelling of Material Separation and Self-Contact with an Adaptive Particle Finite Element Method**

Schewe, Markus (1); Menzel, Andreas (1,2) 15:00
*1: Institute of Mechanics, TU Dortmund university, Germany*
*2: Division of Solid Mechanics, Lund university, Sweden*

We present a Particle Finite Element Method (PFEM) framework for modelling material separation, crack evolution, and complex self-contact in solids undergoing very large deformations. The method targets scenarios where classic finite element technology suffers from mesh distortion and where material failure is governed by shear-dominated mechanisms rather than tensile fracture alone. Typical applications include macroscopic chip formation in machining or abrasive wear, as well as adhesive wear arising in the interaction of rough surfaces on the microscale.

The framework employs a 2D adaptive remeshing strategy based on constrained Delaunay triangulations applied directly to the Lagrangian point clouds representing the bodies. Refinement of the point distribution is achieved through point insertion in zones of high plastic strain, ensuring sufficient spatial resolution of localisation and crack formation. The evolving boundary is reconstructed using an alpha-shape method, which generally can detect local topological changes in the point cloud. For shear-dominated deformation, however, material separation cannot be modelled by geometric detection alone, due to the continuous adaptive mesh regeneration, which heals local point separation before cracks can initiate. Material separation is therefore triggered by a local failure indicator derived from large-strain elastoplasticity, which increases the alpha-shape sensitivity and subsequently results in element removal. This enhanced alpha-shape detection in combination with adaptive remeshing enables modelling of crack initiation and surface evolution in a geometrical manner without predefined cohesive interfaces, smeared damage models or discontinuous Finite Element methods.

Self-contact is modelled through a consistent contact-patch discretisation that is regenerated after each remeshing step. The procedure guarantees that newly formed crack faces interact correctly, preventing interpenetration while preserving the evolving topology. The method therefore allows detection of both inter-body contact and internal self-contact of separating surfaces.

The method is demonstrated for shear-dominated separation of a sinusoidal surface structure, with contact-driven deformation leading to material removal, showing that adaptive PFEM provides an efficient and physically interpretable alternative to classic damage or phase-field formulations.

**Modelling contact of crack faces to study conditions of anticrack propagation**

Hach, Mathis (1); Hopfe, Johannes (1); Schirmer, Arne (1); Mantič, Vladislav (2); Weißgraeber, Philipp (1) 15:20
*1: Chair of Lightweight Design, University of Rostock, Germany*
*2: Grupo de Elasticidad y Resistencia de Materiales, Universidad de Sevilla, Spain*

The concept of anticracks is used to describe localized damage with lateral propagation under compressive loading. Such localized damage can only appear in porous materials where a volume loss mechanism exists. Materials exhibiting this behavior include snowpacks, glass foam, additively manufactured metamaterials and sedimentary rock [1-2]. It has been shown that concepts of classical fracture mechanics can be applied to describe such phenomena and that the behavior is associated

with negative mode-I (mode-I$^-$) stress intensity factors [2]. However, for long anticracks, the collapse surfaces may come in contact again and transfer a portion of the remote compressive loading. Yet only few models of anticracks have been proposed that account for crack face contact and those that exist have been used mainly to analyze snow-mechanics experimental configurations [3]. Until now no general solution for anticracks in large domains exhibiting crack face contact has been developed.

In this work, we provide a nonlinear continuum model for the generalized anticrack based on the canonical example of a Griffith crack. We combine the Westergaard solution for a central crack with an extended Hertzian contact solution by considering an initial gap between the anticrack faces given by the collapse height. The implicit set of equations of contact pressure and contact length is solved by an efficient root search. The stress intensity factors can then be obtained by superposition.

The results of the model show very good agreement with a finite element reference solution. Using this model, we compute nonlinear stress intensity factors for both short and long contact lengths, and convergence in the stress intensity factor for increasing crack lengths is observed. Moreover, the model reveals a compaction window propagating normal to the applied compressive load for large anticrack lengths. Furthermore, the influence of the interdomain on the pressure distribution as well as the stress intensity factor is demonstrated and the effect of an elastic interdomain is considered.

[1] Fletcher, R. C., & Pollard, D. D. (1981). Anticrack model for pressure solution surfaces. Geology, 9(9), 419-424.

[2] Adam, V., Bergfeld, B., Weißgraeber, P., van Herwijnen, A., & Rosendahl, P. L. (2024). Fracture toughness of mixed-mode anticracks in highly porous materials. Nature Communications, 15(1), 7379.

[3] Rosendahl, P. L., Schneider, J., Bobillier, G., Rheinschmidt, F., Bergfeld, B., van Herwijnen, A., & Weißgraeber, P. (2025). The effect of slab touchdown on anticrack arrest in propagation saw tests. Natural Hazards and Earth System Sciences, 25(6), 1975-1991.

**Simulation of crack surface friction within the phase-field method**

Koch, Leonie; Curoșu, Verena; Loehnert, Stefan 15:40
*TUD Dresden University of Technology, Germany*

Cracks and the associated frictional forces that arise under combined compressive and shear loads at the crack surfaces can significantly impact the material behaviour, which is particularly relevant if the load direction changes after the formation of the cracks.

The phase-field method is a powerful method for the simulation of cracks and their propagation, enabling automatic handling of crack propagation, including the detection of the direction and length of the propagation, and it can even capture coalescence and branching of cracks.
However, to the best of the author's knowledge, no generalisable method for the simulation of crack surface friction under combined compressive and shear loads within the phase-field method has been published yet. This contribution might therefore be considered as a first attempt in this direction.

Since the cracks are not modelled discretely in the phase-field method, but are represented by a reduction of the material stiffness, which is applied in a certain width that is determined by the internal length parameter, this represents a particular challenge.

Coulomb's friction law is used for the simulation of crack surface friction, and it is adapted for the calculation of the stick and slip state analogously to elastoplastic models.

The method has been tested with a set of numerical tests showing promising results indicating that the approach has the potential to correctly represent crack surface friction in rather general cases.

Thus the approach can be a valuable contribution to a more accurate modeling of material behaviour and failure within the framework of the phase-field method.

## S03.07: Miscellaneous

Date: March 20, 2026 08:30–10:30
Room: KII, M17.74
Chair(s): Löhnert, Stefan

### # Convex continuum damage models with softening

Lauff, Celine (1); Schneider, Matti (2,3); Schlichting, André (4); Böhlke, Thomas (1) 08:30
*1: Karlsruhe Institut of Technology (KIT)*
*2: Universität Duisburg-Essen*
*3: Fraunhofer Institute of Industrial Mathematics ITWM*
*4: University of Ulm*

Classical local damage models which represent softening behavior come with a serious bottleneck: Their computational response at component level depends on the used mesh, a result of the underlying mathematical ill-posedness of the localization phenomenon implied by softening.
Traditional remedies include non-local or gradient-enhanced formulations which effectively preclude localization by introducing a suitable length scale. However, these formulations come with a few downsides: They are typically rather intrusive into finite element (FE) codes, they are not necessarily well-posed in terms of uniqueness and they do not admit homogenization, i.e., scale transition. The alternative route via adding a dissipative term nullifies the elastic region of the model.

We discuss a damage-modeling approach based on measure theory, i.e., describing the distribution of "damaged mass". Based on the established framework of continuum thermodynamics, the model is formulated by specifying both the free energy and the dissipation in a direct way. The involved potentials are, by definition, convex, and lead to a well-posed mechanical problem. Put differently, the model leads to a mesh-independent response which may be computed in a numerically robust way. Moreover, due to their local nature, these models may be readily integrated into conventional user subroutines of industrial FE codes.

### Convexification-based local continuum damage modeling with damage-softening behavior

Lauff, Celine (1); Schneider, Matti (2); Böhlke, Thomas (1) 08:50
*1: Karlsruhe Institute of Technology (KIT), Germany*
*2: University of Duisburg-Essen, Essen, Germany*

Standard continuum damage approaches use non-local regularization techniques, e.g., additional gradient terms or integral formulations, to ensure mesh-dependent results in the regime of damage-softening [1]. As these countermeasures involve neighbourhood information to compute the mechanical response at a material point, the integration into conventional finite-element codes via user-subroutines is not straightforward. Moreover, the regularization techniques typically involve a length scale parameter, which may be difficult to determine by physical or mathematical means, and are incompatible with multiscale modelling.

To provide a local damage-model, i.e., without any additional damage-gradients, filtered averages or length scale parameters, Schwarz et al. [2] followed an alternative regularization approach, accounting for the mathematical underpinnings of the localization phenomenon. Due to a celebrated result by Morrey, quasiconvexity of the integrand serves as a necessary and sufficient condition for the existence of minimizers of integral functionals, up to additional technical requirements. To guarantee these properties, Schwarz et al. [2] first selected a scalar damage model with damage-rate limitation, ensuring the coercivity of the emerging condensed incremental energy. In a subsequent step, Schwarz et al. [2] proposed to convexify the condensed incremental energy to guarantee the second condition for the existence of minimizers – since every convex function is also quasi-convex.

Whereas Schwarz et al. [2] only introduced an approximation for the damage-minimization process, we derive an analytical formulation of the convex envelope [3]. The presented model shows similarities with the optimal transport theory and prevents localization due to its convex and coercive condensed incremental energy. We discuss the mechanical implications of the damage model and demonstrate the numerical robustness with pertinent computational investigations. In addition, we showcase the mesh-independence of the results and demonstrate the emergence of representative volume elements, essential for homogenization frameworks.

References:
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[2] S. Schwarz, P. Junker, and K. Hackl: Variational regularization of damage models based on the emulated RVE. Continuum Mechanics and Thermodynamics, 33(1), 69-95 (2021).
[3] C. Lauff, M. Schneider, and T. Böhlke: Numerically robust local continuum damage models with softening response via convex relaxation, Submitted (2025).

**Cutting Soft Materials: Mechanics Beneath the Surface**

Moreno-Mateos, Miguel Angel (1); Steinmann, Paul (1,2)

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09:10

Cutting soft materials is a multiphysics process governed by large deformations, interfacial soft fracture, and tool–material contact. Despite its ubiquity, fundamental questions remain: How is energy partitioned between elastic storage, fracture creation, and contact dissipative pathways? How do these mechanisms modulate the stable or unstable transition from indentation to cutting? How do adhesive wear and Coulomb friction compete in controlling cutting resistance? Why do different materials exhibit distinct responses to the same blade?

We combine cutting experiments on three representative soft materials—a hydrogel, an elastomer, and food materials—with a coupled computational framework incorporating cohesive-zone fracture, adhesion, frictional contact, and rate-dependent damping. Experiments reveal material-specific cutting signatures, including abrupt or gradual transitions from indentation to crack initiation and characteristic steady-state cutting regimes.

The model reproduces these behaviors and provides mechanistic insight, showing that adhesive and damping contributions within the cohesive interaction dominate tangential stresses, while Coulomb friction is negligible due to the low normal pressures typical of soft cutting. Simulations further demonstrate that material-specific dissipative parameters govern cutting onset and fracture stability. Together, these results establish a unified framework for soft cutting that links bulk deformation, fracture, and contact dissipation. The combined experimental–computational approach explains why materials with similar stiffness respond differently to the same blade and offers design principles for soft cutting.

Reference:

M.A. Moreno-Mateos, P. Steinmann. “Cutting soft materials: how material differences shape the response”. Accepted, in press in *npj Computational Materials*.

**Predicting Fracture Path In Random Networks**

Shekh Alshabab, Somar; Markert, Bernd; Bamer, Franz

*RWTH Aachen, Chair and Institute of General Mechanics, Germany*

09:30

The complex interplay of geometric disorder and long-range elastic fields is a defining feature of random network materials and poses a fundamental challenge to understanding their fracture behavior. Significant efforts have focused on identifying shear transformation zones as precursors to material

failure. However, their connection to fracture propagation remains largely unexplored. In this study, we utilize Monte Carlo bond-switching simulations to generate two-dimensional amorphous silica networks and investigate their failure mechanisms under athermal quasi-static tensile loading. By analyzing the initial configurations, we map the probability fields of local atomic rearrangements and demonstrate that the eventual fracture trajectory is strongly correlated with the path of maximal activation probability. These results suggest that the failure path in amorphous solids is governed by the configurational landscape of energetically favorable rearrangements

**An improved extended phase-field method for the efficient simulation of fracture**

Curosu, Verena; Loehnert, Stefan 09:50
*Technische Universität Dresden, Germany*

The smeared representation of the crack, as utilized within the phase-field method for fracture, yields significant advantages over discrete methods, such as the extended/generalized finite element method (XFEM/GFEM), regarding the reproduction of complex crack geometries, such as those resulting from crack coalescence and crack branching, especially in 3D. One significant drawback of the method compared to the XFEM/GFEM, however, is the need for a high-resolution discretization by means of a fine mesh or a high polynomial ansatz order in the vicinity of the crack to adequately capture the phase-field, the displacement field and their respective gradients, which increases computational effort.
Within the extended phase-field method (XPFM), the concept of the XFEM/GFEM, extending and adapting the ansatz functions to incorporate information about the expected solution, is applied to improve the reproduction of the phase-field and the displacement field. With this, the aforementioned need for extremely fine meshes or high-order polynomial ansatz functions is overcome. However, the computation of the displacement enrichment within the original version of the XPFM relies on detecting so-called crack points and defining a direction perpendicular to the crack path. This negates, to some extent, the advantage of the non-discrete approximation of the crack in the phase-field method.
In this contribution, an improved version of the XPFM is introduced, in which the displacement field ansatz relies on a distortion of the reference space of the enriched elements. To calculate this distortion, a stiffness-degradation-dependent, and, therefore, phase-field dependent Laplacean problem is formulated and solved for each enriched element on a sub-mesh under incorporation of specific boundary conditions, which ensure the adherence to coordinate properties. On this sub-problem, EAS-type elements are employed to prevent an overly stiff behaviour of the solution due to locking. Since this reference-space distortion is directly coupled to the stiffness degradation, no additional discretization of the crack geometry is required, thereby preserving the advantage of the smeared representation of the crack. As a result, the method is more versatile than its predecessor and can more easily account for crack branching and coalescence.
Within the contribution, the new XPFM approach is presented, including the transformed phase-field ansatz, the enriched displacement field ansatz and the calculation of the distorted reference coordinates. Several examples are shown to display the efficacy of the method.

**Computationally efficient phase field models of fracture based on novel monolithic arc-length methods**

Rörentrop, Felix; Langenfeld, Kai; Mosler, Jörn 10:10
*TU Dortmund University, Germany*

The computational modelling of brittle fracture has been a long-standing challenge in computational mechanics and remains highly relevant today. For example, rate-independent phase-field models of brittle fracture are well known to exhibit unstable, time-discontinuous crack evolution caused by the non-convexity of the underlying energy - also known as brutal crack growth. Such unstable crack growth poses severe challenges for standard numerical solvers [1]. A widely used remedy is the reparametrization of (pseudo-)time via arc-length techniques. In this contribution, existing arc-length methods for phase-field fracture are revisited and novel methods are elaborated. The central result is a reinterpretation of the Efendiev & Mielke scheme, originally developed to approximate Balanced-Viscosity solutions, as a non-standard arc-length method [2]. Based on this insight, a novel monolithic

solver is proposed. Numerical examples are presented, showing the novel arc-length schemes to be capable of robustly capturing unstable crack growth while significantly improving computational efficiency compared to existing numerical schemes.

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[2] F. Rörentrop, K. Langenfeld, J. Mosler. "A computationally efficient monolithic arc-length method for phase-field models of fracture based on the Efendiev & Mielke scheme". SSRN, https://doi.org/10.2139/ssrn.5960260

## S04: Structural mechanics

Organizer(s): Sauer, Roger *(Ruhr University Bochum)*
Klinkel, Sven *(RWTH Aachen University)*

## S04.01: Structural mechanics

Date: March 17, 2026 08:30–10:30
Room: KI, M11.32
Chair(s): Klinkel, Sven
Sauer, Roger

### A stabilization technique based on a Taylor series expansion for virtual elements

Pacolli, Njomza (1); Kehls, Jannick (1); Reese, Stefanie (2); Holthusen, Hagen (3) 08:30
*1: Institute of Applied Mechanics, RWTH Aachen University*
*2: University of Siegen, Germany*
*3: Institute of Applied Mechanics, University of Erlangen-Nuremberg*

Stabilization techniques combined with reduced integration are widely used in numerical methods to overcome locking phenomena. In the context of finite element methods, approaches such as enhanced assumed strain formulations (EAS) [1] are often coupled with stabilization techniques to overcome specific types of locking, including volumetric and shear locking. This combination improved the performance of low-order finite element formulations while addressing the downsides of reduced integration.

The virtual element method (VEM) has emerged as an extension to the finite element method, capable of handling arbitrary polygonal and polyhedral meshes, enabling flexibility in mesh generation and refinement [2]. This makes VEM well suited for problems involving distorted, non-convex and irregular meshes. Similar to reduced integration, VEM formulations require stabilization to avoid rank deficiencies and ensure numerical consistency. A variety of stabilization methods have been proposed to address these challenges, e.g. [3].

In this contribution, a stabilization technique based on a Taylor series expansion of the constitutive quantities in combination with reduced integration is presented and investigated, with a particular focus on their application within the framework of the VEM. This has already been explored for regular elements [4] and is now expanded to polygonal meshes.

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### A scaled boundary finite element formulation for static and dynamic analysis of Reissner-Mindlin plates

Hellers, Anna; Reichle, Mathias; Klinkel, Sven 08:50
*RWTH Aachen University, Germany*

In the analysis of thin plates, finite elements based on Kirchhoff-Love or Reissner-Mindlin plate theories are commonly employed. While Kirchhoff plates require a $C^1$-continuity of the shape functions, Reissner-Mindlin formulations impose less restrictive continuity requirements but can experience transverse shear locking in the thin plate limit, significantly compromising the effectiveness of the formulation. This drawback has led to the development of various remedies, such as discrete shear

gaps and assumed natural strains [1]. However, most techniques are limited to standard triangular and quadrilateral finite elements.

Meanwhile, the growing complexity of the designs has recently increased the interest in polygonal finite elements, such as Virtual Element Methods, barycentric coordinates and Scaled Boundary Finite Element Methods. These methods significantly simplify the domain discretization, especially in cases involving local mesh refinements and quadtree meshes where automatic handling of hanging nodes is possible. Consequently, locking remedies applicable to elements with varying numbers of nodes are required.

This work presents a fully discretized Scaled Boundary Finite Element [2] for Reissner-Mindlin plate theory, where the analytical solution in the scaling direction from the original semi-analytical approach is replaced by a weak approximation using low-order shape functions. The issue of transverse shear locking is addressed through an assumed natural strain approach tailored for application on polygonal Scaled Boundary Finite Elements [3]. The effectiveness of the formulation is demonstrated through numerical examples of static analysis, followed by an analysis of free vibrations and their eigenmodes.

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[2] Klinkel S, Reichel R. A finite element formulation in boundary representation for the analysis of nonlinear problems in solid mechanics. Comput Methods Appl Mech Eng. 2019; 347: 295-315

[3] Hellers A, Reichle M, Klinkel S. A polygonal Reissner-Mindlin plate element based on the scaled boundary finite element method. Comput Mech, in press

**Polyhedral elements based on scaled boundary parametrizations – a comparative study of semi-analytical vs IGA-based formulations**

Pasupuleti, Ajay Kumar (1); Nattoji Shara, Sharath (1); Parrales, David Teran (2); Chasapi, Margarita (2); Birk, Carolin (1)

*1: University of Duisburg-Essen, Germany*
*2: RWTH Aachen University, Germany*

09:10

Polytope elements provide great flexibility with respect to meshing of complex and evolving geometries. They have thus gained popularity in the context of fracture simulation and for modelling physical processes in highly heterogeneous domains, for example. In 2D, polygon element formulations based on e.g. the virtual element method (VEM), Wachspress shape functions, or the scaled boundary finite element method (SBFEM) have been proposed. Quadtree meshes, that consist of square elements only are a special case of polygon meshes. These can be created automatically from digital images and lend themselves to adaptive refinement. The ubiquitous hanging nodes problem is addressed straightforwardly using the polygon element formulations mentioned above.

While polygon elements have been studied in detail and a comparison of various formulations has been published, polyhedral elements have received less attention. In 3D, elements with an arbitrary number of faces can be constructed using scaled boundary parametrizations. Here, only the surface of a polyhedral domain is meshed using two-dimensional surface elements, while the interior is described by scaling the geometry of the boundary. This procedure has originally been suggested in the context of SBFEM, where formulating a weak statement with respect to the circumferential directions yields an ordinary differential equation with respect to the remaining radial direction, which can be solved for special cases such as linear elasticity. Here, the polyhedral faces are typically disretized using standard finite elements or polygon elements based on Wachspress shape functions. The SBFEM facilitates solutions on octree meshes, which excel in rapid mesh size transition. On the other hand, octree meshes lead to stair-case approximations of geometric boundaries. As an alternative, IGA-based polyhedral elements have been proposed. While using the same idea of scaling the surface discretization, the resulting ordinary differential equation is solved numerically, that is, a numerical

approximation of the solution in both circumferential and radial direction is obtained. Moreover, isogeometric analysis is used both in that solution process and in discretizing the boundary. Thus, highly accurate representations of curved geometries are obtained.

This presentation provides a comparative study of polyhedral element formulations based on scaled boundary parametrizations of the boundary. Specifically, the semi-analytical SBFEM and its IGA-based variant are discussed. Both methods are evaluated in terms of stability, convergence behavior and flexibility in the context of linear elasticity by applying them to benchmark examples and by comparing the results using measures such as error norms, convergence rates and deformations.

**An enhanced approximate dual basis functions-based static condensation approach for a mixed isogeometric plate formulation**

Dornisch, Wolfgang; Stammen, Lisa
*RPTU Kaiserslautern-Landau, Germany*

09:30

Within isogeometric analysis, the geometry is represented employing non-uniform rational B-splines that are constructed based on knot vectors. Depending on the underlying geometry and the employed approximation order, the knot vectors can possess different continuities. This is known to enable higher accuracy, due to the exact preservation of the structure's geometry during the analysis, as these curves are also employed as basis functions for the interpolation of the unknown quantities.

A common method to tackle certain locking phenomena is to employ mixed formulations, where quantities from multiple physical fields are interpolated independently. Furthermore, this allows the selection of adequate (selectively reduced) approximation orders for the different physical fields. As the introduction of additional unknowns results in an increased computational effort, commonly, static condensation procedures are employed to eliminate these parameters without reducing the increased accuracy of the mixed formulation.

In previous investigations, it has been shown that the calculation of the inverse of the sub-matrix associated with the additional parameters, which is required for standard static condensation procedures, can be prevented by employing (approximate) dual basis functions for the interpolation of the corresponding virtual parameters in conjunction with an adequate factorization of the relevant governing equations and subsequent row-sum-lumping.

Within this contribution, deteriorated convergence rates, which are observed when solving problems involving internal knots of limited continuity within the discretization by such efficient dual formulations, are tackled by performing an appropriate reduction of internal continuity while employing enhanced approximate dual basis functions. Numerical examples show that the optimal convergence rates can be obtained in all cases when considering the guidelines of this contribution.

**Reducing the Variational Index for a Hierarchic Family of Structural Formulations**

Mitruka, Tarun; Bischoff, Manfred
*University of Stuttgart, Institute for Structural Mechanics, Germany*

09:50

Transverse shear locking, characterized by the appearance of parasitic shear forces and underestimated displacements, occurs in finite elements based on shear-deformable structural formulations, typically for slender structures. Classically, these models involve the displacements and total rotations of the cross-sections as unknown quantities. While numerous remedies exist to alleviate locking in the finite element method (FEM), with emerging discretization methods like meshless methods, isogeometric analysis (IGA), scaled boundary FEM, etc., revisiting these remedies becomes a necessity. To circumvent this process, a family of so-called hierarchic formulations was developed. The idea is to use a shear-rigid Kirchhoff-type model as a base model, to which either shear rotations [1] or shear displacements [2] are hierarchically added and used as unknowns, instead of the total rotations. The resulting formulations were found to be intrinsically free from transverse shear locking, i.e., they are locking-free independent of the discretization method. However, since a Kirchhoff-type model is used as a base model, higher derivatives appear in the weak form, requiring smoother basis functions for

the unknowns, which is uncommon for shear-deformable models and may be considered a major obstacle for widespread application.

In this work, an overview of hierarchic formulations to mitigate transverse shear locking is first presented. Next, a mixed method is introduced that uses the change in curvature as an additional unknown and aids in reducing the variational index of the underlying weak form. This facilitates the usage of, for example, standard Lagrange shape functions, while preserving the hierarchic nature. The advantages and limitations of this method are then briefly commented upon, highlighting comparisons with some mixed methods from the literature. Numerical examples, in the context of FEM and IGA for geometrically linear beam, plate, and shell problems, are finally presented. The main focus of the work is on developing a mixed method that enables reducing the variational index of the weak form in hierarchic formulations.

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[2] Oesterle, B., Ramm, E., Bischoff, M., 2016. A shear deformable, rotation-free isogeometric shell formulation. Computer Methods in Applied Mechanics and Engineering 307, 235–255.

**Fully Nonlinear Analysis of Triangular Shell Elements for Thin-Walled Applications**

Sousa, Cinthia Andreia G. (1,2); Vorwerk, Maximilian (1); Pimenta, Paulo M. (2); Schröder, Jörg (1)

*1: University of Duisburg Essen, Germany*
*2: Polytechnic School at University of São Paulo*

10:10

The geometric flexibility of triangular shell elements and their suitability for irregular meshes contribute to their attractiveness for modeling components such as curved panels, slender shells, and lightweight structural assemblies. For this reason, triangular shell elements play a significant role in the numerical analysis of thin-walled structures that are encountered in aerospace, energy, and manufacturing applications. Admittedly, despite their extensive adoption, different triangular formulations can exhibit distinct behaviors depending on their underlying kinematic and numerical characteristics. This underscores the necessity for a more comprehensive investigation of their performance in nonlinear environments.

This work investigates the performance of triangular shell elements within a fully nonlinear analysis framework, focusing on formulations based on Reissner-Mindlin kinematics. To this end, displacement-based triangular shell elements with enhanced rotational treatment is considered, emphasizing their suitability for nonconforming meshes and geometrically intricate domains. The study considers formulations capable of capturing finite strains, large displacements, and large rotations, with particular attention to the treatment of rotational fields, strengthening numerical stability and accuracy relative to classical parametrizations.

A set of representative nonlinear shell problems is employed to explore how various triangular formulations respond under severe deformation states. This approach enables the identification of characteristic trends, strengths, and limitations across different element behaviors without restricting the assessment to a single performance indicator. The results demonstrate the capacity of advanced triangular elements to robustly capture complex deformation patterns, particularly in scenarios involving irregular meshes, geometric intricacies, and large-scale nonlinear effects.

**S04.02: Structural mechanics**

Date: March 17, 2026 16:30–18:30
Room: KI, M11.32
Chair(s): Oesterle, Bastian
Klinkel, Sven

**Data-based estimation of the critical time step size for explicit time integration in dynamics**

Schilling, Maximilian; Reinken, Lisa-Marie; Bischoff, Manfred 16:30
*University of Stuttgart, Germany*

Stability of explicit time integration in structural dynamics, e.g. using finite elements, is limited by a critical time step. However, computing it exactly by solving the corresponding eigenvalue problem is too expensive. Therefore, there are several approaches to estimate the critical time step, many of them through an estimation on the element level. A popular and inexpensive approach is to estimate the critical time step via heuristic formulas based on a characteristic element length. The estimate is obtained by dividing it by the wave speed. For instance, the characteristic length of a 2D quadrilateral solid element can be calculated by the element area divided by its longest side or its longest diagonal. However, the resulting estimates are usually non-conservative, which necessitates a safety factor to prevent instabilities. For other element types, for instance 3D tetrahedral elements, these heuristic estimates are even less accurate. More accurate time step estimators can be derived by utilizing data sets of relevant element shapes within a data-integrated machine learning approach. Numerical examples confirm that this new approach outperforms state of the art estimators, allowing for larger time steps and thus reducing computation time. It is an example for applying methods of machine learning to computational mechanics in a way that exploits the efficiency of neural networks while avoiding the downside of relying on black-box approaches.

**Determination of the mass moment of inertia by surface integration**

Hartmann, Stefan; Ewougsi Tekeu, Christian-Lionel 16:50
*Clausthal University of Technology, Germany*

Gauss's integral theorem, i.e. the divergence theorem, can be applied to convert a volume integration to a surface integration. With a suitable integrand, it is known that the volume and center of mass can be determined by surface integration. In this contribution a suitable integrand is provided for which the mass moment of inertia tensor can be calculated through surface integration alone. A similar procedure is used to calculate area moments of inertia and moments of deviation.
In addition to theoretical derivations, this concept is applied to surface triangulation, enabling CAD programs to quickly determine moments of inertia. However, this method produces asymmetrical mass moment of inertia tensors in certain surface discretizations, which can be resolved by employing symmetrization. Accuracy investigations follow the computations for particular geometries, revealing good agreement with analytical approaches. Finally, similar analogies are demonstrated for the moment of area matrix.

**On theoretical aspects of intrinsically selective mass scaling for thin-walled structures**

Reinhart, Sven; Oesterle, Bastian 17:10
*Hamburg University of Technology (TUHH), Germany*

For explicit time integration methods in structural dynamics, the critical time step size depends on the highest frequency of the discretized system. Mass scaling methods can be used to reduce these high frequencies and, thus, to increase the critical time step size by increasing inertia. But this typically comes at the cost of compromising accuracy. For shear deformable beam, plate and shell formulations, the time step is usually limited by the highest transverse shear frequencies, which are often of minor importance for the overall structural response.

Primal hierarchic structural element formulations [1, 2] are based on a reparametrization of the kinematic equations. The parametrization using transverse shear parameters allows a selective scaling of transverse shear frequencies in a simple manner, while bending and membrane frequencies are practically not affected. The novel concept of intrinsically selective mass scaling (ISMS) [3, 4] features high accuracy. Unlike other selective mass scaling techniques, ISMS preserves the diagonal structure of lumped mass matrices.

In this contribution, we present recent research on theoretical aspects of ISMS for hierarchic structural element formulations. We show that ISMS exactly preserves both linear and angular momentum. We

underline the high accuracy and the selectivity of ISMS by systematic analyses of scaled frequency spectra using Rayleigh quotients and show recent results on time step estimation.

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**On efficiency, accuracy and robustness of selective mass scaling methods for thin solid and solid-shell elements**

Hoffmann, Moritz; Oesterle, Bastian 17:30
*Hamburg University of Technology, Germany*

The critical time step size in explicit dynamics depends on the highest discrete frequency, which is, for discretizations composed of thin solid or solid-shell elements, typically related to thickness stretch modes [1].

Selective mass scaling (SMS) methods aim at increasing the critical time step size by scaling down the highest frequencies while preserving accuracy in the lower part of the frequency spectrum. But the use of SMS typically comes at the cost of non-diagonal mass matrices and the need for using iterative solvers in each time step. The overall efficiency of SMS depends on the number of time steps, the numerical cost of overhead associated with SMS per time step, and the desired level of accuracy.

In this contribution, we present recent results on the extension of our novel SMS method [2] to solid-shell elements. We compare our method with SMS concepts from literature with respect to efficiency, accuracy and robustness in both spectral and transient problems.

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**Active Learning–Based Experimental Design for Nonlinear Structural Dynamics Using Physics-Guided Neural Networks**

Shine, Yadukrishnan (1); Pei, Jin-Song (2); Altay, Okyay (1) 17:50
*1: Chair of Structural Analysis, Department of Civil Engineering, University of Siegen, Germany*
*2: School of Civil Engineering and Environmental Science, Gallogly College of Engineering, University of Oklahoma, USA*

Understanding and predicting the behavior of structural systems is a central objective across many engineering disciplines, especially when these systems are exposed to complex dynamic loads. As modern structures increasingly incorporate nonlinear components and demand high-performance operation, traditional modeling and experimental practices often struggle to capture the full range of system behaviors. Data-driven methods have emerged as promising tools for bridging this gap, but they depend heavily on the quality and diversity of experimentally acquired data. This motivates the

development of testing strategies that deliberately seek out the most informative data rather than relying on fixed or intuition-based procedures.

In response to this need, our previous research developed an active learning framework to guide experimental design by integrating force-state mapping with a feedforward neural network, using the model's accuracy as an optimization criterion. By applying a pattern-search strategy to find the optimal experimental parameters, the approach steered the system toward the most informative responses, reducing the number of experiments by more than a factor of three relative to conventional unsupervised data sampling. However, finding a matching network architecture and determining its initial weights and biases remained an open question. While using ensemble training of a set of different network architectures offered a temporary solution, it came at the cost of excessive computational effort and reduced robustness.

The present study advances this framework by incorporating physics-guided neural networks. In this approach, the network architecture and its initialization are determined using a library of prototypical formulations extracted from the governing equations of typical nonlinear systems. By choosing and combining these formulations, an optimal representation is established that mitigates bias error, constrains model complexity through a predefined architecture, and produces training dynamics that require significantly less effort. Importantly, eliminating model bias error also smooths the unknown loss surface, enabling the active learning algorithm to explore the space of experimental parameters more efficiently and converge more rapidly toward informative testing regimes.

The physics-guided framework is demonstrated on a Duffing oscillator, a canonical nonlinear system whose resonant frequency shifts with increasing amplitude due to its cubic stiffness nonlinearity. Despite the complexity introduced by this amplitude-dependent behavior, the proposed approach successfully identifies optimal excitation parameters that generate highly informative data for model development. Comparative results show clear improvements in efficiency and robustness relative to the previous version, highlighting the advantages of integrating physical knowledge into data-driven experiment design.

**A Residual-Based Variational Approach to Global and Goal-Oriented Reanalysis**

Materna, Daniel 18:10
*OWL University of Applied Sciences and Arts, Germany*

In this contribution, a global and goal-oriented reanalysis framework is proposed for efficiently predicting changes in primal and dual solutions as well as selected quantities of interest caused by structural modifications, including variations in shape, topology, or material properties. This work is based on a rigorous and variationally consistent derivation of the reanalysis formulation, which establishes a residual-based framework.
Starting from the variational form of the governing equations, the residuals associated with modified structural configurations are systematically derived and decomposed into incremental contributions. This incremental residual decomposition provides a basis for updating the structural response under successive design changes and enables a consistent extension to both linear and nonlinear reanalysis problems. The formulation relies on primal and dual problems and does not require derivatives with respect to the design variables, which significantly facilitates its implementation in existing finite element codes.
The resulting global and goal-oriented reanalysis approach is particularly well suited for applications involving a large number of design iterations, such as structural optimization, reliability analysis, and structural damage assessment. In such applications, repeated solutions of the full state problem and

the evaluation of quantities of interest lead to substantial computational costs. By exploiting the proposed variational residual framework, the overall computational effort in numerical simulation with structural modifications can be reduced.

## S04.03: Structural mechanics

Date: March 18, 2026 08:30–09:30
Room: KI, M11.32
Chair(s): Sauer, Roger
Gudžulić, Vladislav

### Nonlinear analysis of steel-concrete composite beams with steel connectors and/or adhesive bonding

Kuczma, Bozena; Kuczma, Mieczyslaw 08:30
*Poznan University of Technology, Poland*

Composite structures of steel and concrete offer numerous advantageous properties, making them optimal for structural material design. This solution is based on the principle that steel should be placed in regions under tension while concrete is used in areas dominated by compression. The interaction between the steel and the concrete is critically important.

In this talk, we will develop a mathematical model for composite beams with deformable connections between the steel girder and the concrete plate, based on our laboratory experiments. We considered different types of steel-concrete connections using steel shear-headed studs and/or flexible and stiff structural adhesives. The tests were conducted on steel-concrete beams, their representative fragments, and single-material coupons. Measurements of quantities of interest (displacements, strains) were obtained using the strength machine control system, a 3D optical non-contact measuring DIC system (Aramis/Pontos), and a large number of traditional sensors and LVDTs.

The evolutional boundary value problem governing the deformation process of the composite beams is formulated as a system of equations and inequalities that reflect the nature of the elasto-plastic behaviors of steel, concrete, connectors, and unilateral contact conditions, or equivalently, in a weak form as a complex variational inequality. The finite element approximation and an explicit time-stepping scheme are used, allowing us to solve the variational inequality incrementally as a sequence of complementarity problems. Results of numerical simulations of the experimentally tested beams will be presented, showing good agreement between theory and experiment.

### Comparison of numerical simulation using Particle finite element method and experiments of Polymeric composite structures

Kadam, Paras (1); de Payrebrune, Kristin M. (1); Scheunemann, Lisa (2) 08:50
*1: RPTU University Kaiserslautern-Landau, Germany*
*2: RWTH Aachen University, Aachen*

Modeling large deformations in compliant structures presents well-known challenges for conventional Finite Element Method (FEM) formulations, which often suffer from mesh distortion and numerical instability. These issues become more pronounced in systems with spatially varying material properties. To address these limitations, the Particle Finite Element Method (PFEM) offers a robust alternative. In PFEM, the domain is represented by a set of particles and a finite element mesh is subsequently generated from these particles to compute the solution of the governing equations **[1]**. At the end of a time step, this mesh can be discarded and regenerated, enabling the method to avoid the progressive degradation of mesh quality. Through its Updated Lagrangian formulation and continuous remeshing strategy, PFEM reduces mesh distortion and maintains element quality under severe geometric changes, making it well suited for problems involving complex deformation patterns and material heterogeneity **[2]**.

In this contribution, PFEM will be used to model the mechanical behavior of polymeric materials. Polymeric materials are widely employed across various engineering domains, including soft robotics, flexible mechanisms, vibration-damping components, and compliant structural devices where large

deformation capacity and nonlinear mechanical behaviour are essential. Many of these structures incorporate intentionally heterogeneous material distributions, consisting of regions of base silicone alongside modified formulations or composite variants **[3]**.

Tensile simulations are carried out on specimens composed of alternating polymeric segments, each characterised by distinct material parameters. A hyperelastic material model is employed to account for the large, recoverable strains and inherent nonlinear stress–strain behaviour of polymers **[4]**. To assess the predictive capability of the numerical model, tensile experiments are conducted on specimens fabricated with the same material layout, allowing direct comparison with the simulation results.

**References -**

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**A Generalized Computational Framework for Shakedown Analysis of Orthotropic Materials**

Vafadari, Reza; Veludandi, Lavakumar; Ochoa Ontiveros, Lilian Aurora; Simon, Jaan-Willem 09:10
*Bergische Universität Wuppertal, Germany*

Shakedown analysis offers a rigorous theoretical and computational basis for establishing the long-term load-bearing capacity of structures subjected to repeated or variable loading. While classical shakedown formulations are well established for isotropic materials, their extension to orthotropic and fibre-dominated materials remains comparatively underexplored, despite the increasing use of such materials in paper engineering, composites, laminated structures, and bio-inspired systems. The present work develops a comprehensive computational framework for the shakedown analysis of orthotropic materials.

The methodology incorporated a fully orthotropic linear elastic constitutive model together with an anisotropic yield criterion, implemented in a way that both the elastic domain and the yiels surface rotate. This ensured that direction dependent stiffness and yielding mechanisms are captured accurately in the global response. The analysis adopted shakedown formulation, where admissible self equilibrated stress fields are obtained through a sequence of finite element response evaluations and convex optimization steps. Finite element response snapshots are generated in Abaqus, whereas the optimization problem governing the construction of the shakedown domain is solved using Gurobi. The framework further integrates automated post-processing to evaluate normalized load factors, visualize residual stress fields, and construct shakedown domains.

The proposed approach is demonstrated on an orthotropic material. Numerical investigations reveal that material anisotropy substantially distorts the shakedown domain, even under geometrically symmetric conditions. Specifically, fiber orientation strongly influences the domain's curvature, load-interaction characteristics, and ultimate collapse mechanisms. These findings highlight the necessity of anisotropy consistent formulations when assessing long-term performance of fiber-reinforced or layered materials.

Overall, the study provides a rigorous, programmable, and extensible framework for shakedown analysis of orthotropic materials. It lays the groundwork for future integration with experimental calibration, nonlinear kinematic hardening, multi-scale modelling, and probabilistic assessment of structural robustness under variable loading.

## S04.04: Structural mechanics

Date: March 18, 2026 14:00–16:00
Room: KI, M11.32
Chair(s): Wackerfuss, Jens
Neu, Gerrit Emanuel

### A fully nonlinear space-time finite element formulation for geometrically exact beams

Steinbrecher, Ivo (1); Humer, Alexander (2) 14:00
*1: Universität der Bundeswehr München (UniBw), Germany*
*2: Johannes Kepler Universität (JKU), Linz, Österreich*

The dynamic simulation of slender structures such as beams plays a key role in many engineering applications, including aerospace structures, flexible robotics, and biomechanical systems. Conventional approaches typically rely on spatial discretization using the finite element method (FEM) combined with time-stepping schemes, such as the Newmark algorithm. In contrast, space-time finite element formulations apply FEM simultaneously in both space and time, resulting in a single system that represents the entire dynamic evolution of the problem.
While space-time formulations generally lead to larger algebraic systems, this aspect is not the focus of the present work and can be addressed using suitable linear solvers and preconditioning techniques. Instead, the advantages of the space-time approach are emphasized, including flexible time discretization, natural compatibility with adaptive finite element strategies, potential for parallel-in-time computation, and a straightforward treatment of changing material domains.
Building on recent developments in space-time finite element methods for solid mechanics, we present a fully nonlinear space-time formulation for three-dimensional geometrically exact Simo-Reissner beams. We employ a mixed-formulation in which displacements and velocities are discretized independently. This allows for a straightforward imposition of initial and boundary conditions, while also providing freedom in the choice of interpolation spaces. To enhance numerical stability and robustness, a residual-based stabilization technique is used.
The beam is modeled as a Cosserat continuum, requiring both position and orientation fields on the space-time surface to be treated as unknown fields. To consistently handle finite rotations, we employ a nodal rotation (pseudo-)vector based description of the orientation field. The rotational interpolation follows established schemes, ensuring objectivity. In the final discretized space-time problem, each finite element node possesses twelve degrees of freedom: translational displacements, rotational vectors, translational velocities, and material angular velocities.
Among the main topics addressed in this talk are the development of a fully nonlinear space-time finite element formulation for geometrically exact beams, as well as a discussion of the formulation's key features, such as the consistent treatment of finite rotations. Selected qualitative and quantitative examples are presented to highlight the accuracy and objectivity of the method, underlining its potential for real-world applications in structural dynamics. Furthermore, the advantages of the space-time approach in the context of changing material domains are demonstrated.

### Transitioning from 3D solid to classical beam kinematics

Klarmann, Simon (1); Wackerfuß, Jens (2); Klinkel, Sven (1) 14:20
*1: Chair of Structural Analysis and Dynamics, RWTH Aachen University, Germany*
*2: Institute of Structural Analysis, University of Kassel, Germany*

Modeling load-bearing structures consisting of components with different dimensionality requires efficient models in order to represent the overall mechanical behavior. For slender components, beam elements offer an efficient way of representing the load-bearing properties of the structure, but they

are unable to capture local effects, such as stress concentrations at bearings or in joint areas. To improve the quality of the results, it is desirable to consider these parts using a 3D solid model. This gives rise to a mixed-dimensional model consisting of beam and solid models. To establish the link between them, a transition zone is introduced which is able to link the models based on different kinematic assumptions, namely the solid's classical displacement field with the three translations and three rotations of the beam model.
In the context of the finite element formulation, the transition zone is discretized using special finite transition elements, whose derivation is a non-trivial task. The classical beam assumption that a plane cross-section remains plane causes severe deterioration of the stress field at the boundary. This results in a significant overestimation of the stiffness of the structure, especially with respect to torsion and shear. Furthermore, normal and bending stiffness are affected due to the missing in-plane deformation of the cross-section suppressing the lateral contraction due to Poisson's ratio. To overcome this limitation, the beam kinematics are enriched by a warping function or, more generally, by a displacement field describing arbitrary in- and out-of-plane deformations of the cross-section. This contribution presents a finite element formulation for the transition zone between solid and beam elements. In this formulation, the aforementioned general deformation function of the cross-section is embedded directly into the element. It is important to note that no a priori determination of the general deformation function is required. Instead, it enters the formulation as an additional displacement field that becomes part of the unknowns and is determined automatically during the usual finite element solution process. As a result, the proposed element formulation for the transition zone is similar to a classical 3D solid element, while enabling the connection to a beam element. Numerical examples demonstrate the performance of the proposed element formulation. Benchmark tests confirm the quality and accuracy of the results. The element formulation leads to accurate stress states within the transition zone for arbitrary cross-sections, as long as it is applied to parts of the model in which the beam theory is valid.

**On the simultaneous analysis of Kirchhoff beams embedded in a two-dimensional bulk domain**

Neumeyer, Jonas; Kaiser, Michael Wolfgang; Fries, Thomas-Peter 14:40
*Graz University of Technology, Austria*

Our contribution presents a mechanical model and numerical method for the simultaneous analysis of curved shear-rigid beams, i.e., Kirchhoff beams, which are geometrically defined via level sets over a two-dimensional bulk domain. This approach follows previous work for ropes and membranes [3], as well as Timoshenko–Ehrenfest beams [4] and Reissner–Mindlin shells [5]. The additional challenge for Kirchhoff beams is found in the increased continuity requirements of the mechanical model. The geometry is defined implicitly through a level-set function, such that each isoline implies an individual beam. Geometric quantities and surface differential operators are defined in the frame of tangential differential calculus [1, 2], hence, they are coordinate-free and apply to implicit geometry descriptions. From a numerical perspective, simulations of Kirchhoff beams involve second-order derivatives in their displacement-based weak form and therefore require $C^1$-continuous discretizations. To overcome this limitation, we adopt a mixed-hybrid formulation, as outlined in [6], in which the moment tensor is introduced as an additional primary unknown. This reduces the continuity requirements to $C^0$, enabling the use of classical Lagrange elements, but also increases the number of degrees of freedom considerably in the context of FEM. A hybridization scheme breaks the inter-element continuity of the moment tensor field and reinforces it weakly using a Lagrange multiplier defined only on element interfaces. This allows for an element-wise static condensation of the field of the moment tensor, yielding a computationally efficient formulation. Several test cases verify the accuracy and higher-order convergence of the proposed method.

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[6] J. Neumeyer, M.W. Kaiser, T.P. Fries, Higher-Order, Mixed-Hybrid Finite Elements for Kirchhoff–Love Shells, *Int. J. Numer. Methods Eng.*, **126**, e70175, 2025.

**Formulation and verification of multi-point constraints to enforce beam kinematics in volumetric FE-simulations of beam-like structues**

Boungard, Jonas; Wackerfuß, Jens 15:00
*University of Kassel, Germany*

When simulating complex slender structures with finite elements, one can either use a computationally efficient beam model or a more detailed and precise continuum model. The former relies on kinematic assumptions that restrict the possible deformations. This leads to a computationally efficient model due to the reduced set of parameters, i.e. the kinematics of the reference axis. While these assumptions allow for a drastic reduction in computational complexity, they also act as kinematic constraints. A beam model inherently satisfies these constraints, but when its results are compared to a more detailed continuum model without constraints, deviations can be observed. In many cases, these deviations remain within acceptable limits, and beam models provide an accurate and efficient representation of the structural behaviour. Yet, there are scenarios where the standard kinematic assumptions are ill suited, leading to significant errors.

Although this phenomenon is well known, no method has been developed to quantify the influence of the kinematic assumptions on the local and global structural behaviour. Such a method is of great interest because it allows the adequate selection of kinematic assumptions for each part of the structure. In order to develop such a method, we want to compare the results of three models: (1) classical beam model following Euler-Bernoulli hypothesis, (2) a continuum model without additional constraints, serving as a reference solution, (3) a continuum model incorporating multi-point constraints to enforce the kinematic assumptions.

Motivated by this, the aim of this talk is to find the correct multi-point constraints that need to be employed in the continuum model to enforce the three kinematic assumptions of Euler-Bernoulli hypothesis: (i) plane cross-section remains plane, (ii) cross-section remains perpendicular to the beam's reference axis, (iii) no stresses in thickness direction. Preliminary investigations show that the third assumption can be translated into different multi-point constraints depending on the specific interpretation. Thus, in the talk, we compare different constraint formulations on the basis of several numerical examples. This allows for the verification of the correct multi-point constraints. Since a large number of nonlinear constraints is introduced, an efficient master-slave elimination scheme is employed for their handling [1,2]. This approach reduces computational cost while maintaining accuracy.

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[2] Boungard, J. and Wackerfuß, J.: *Extension of constraint methods – identification, elimination and handling of redundant and contradictory multi-point constraints*. Submitted.

**Multiscale modelling of hyperelastic shell structures with physics-augmented neural network constitutive models**

Schommartz, Jasper O. (1); Klein, Dominik K. (1); Gruttmann, Friedrich (2); Weeger, Oliver (1) 15:20
*1: Institute Cyber-Physical Simulation, Technical University of Darmstadt, Germany*
*2: Institute for Mechanics, Technical University of Darmstadt, Germany*

Multiscale finite element schemes enable the simulation of arbitrary microstructures within the Mindlin–Reissner shell theory. However, the FE2 approach drastically increases computational cost in the finite-strain case, undermining a main benefit of using shell formulations. Neural network (NN)-based surrogate constitutive model for shells can help to overcome this drawback by moving from a concurrent to a more efficient, sequential multiscale approach.
In the present work, we formulate a thermodynamically consistent NN-based shell constitutive model, focusing on hyperelasticity. A feed-forward NN is used to model the strain energy per unit area as a function of the shell strain measures. The NN potential is complemented by two terms that ensure stress and energy normalization, respectively. Finally, we enforce the constitutive scaling law for hyperelastic shells in the NN model formulation, enabling the representation of different shell thicknesses without additional training data. The model is trained and validated using data from homogeneous and inhomogeneous shell representative volume elements.

**Modelling of sparse lightweight composite designs using a geometrically discontinuous approach**

Kühner, Paul T.; Habera, Michal; Zilian, Andreas 15:40
*University of Luxembourg*

Carbon fibre reinforced polymers (CFRPs) enable lightweight, high-performance, sparse designs. The sparsity of these composite structures amplifies their complex behaviour, creating a challenging mechanical response landscape. We present a model for an additively manufactured, wound CFRP truss structure composed of connection points ("anchors") and one-dimensional members ("strings"). Anchors are attached to an external surface undergoing assumed deformation. Given the high stiffness contrast, anchors are treated as rigid volumes connected by one-dimensional strings. For the material model of the strings, we rely on a geometrically nonlinear (finite deformation), bimodular elastic formulation.

Connectivity information, between strings and anchor volume, translates to a mesh layout consisting of topologically one-dimensional cells, with facets representing the anchor volume's centre points. Additionally, offsets of start- and end points of the strings from the centres are incorporated. Those are superimposed via discontinuous parameters, allowing for the freedom to model multiple strings on a single (topological) anchor point, while allowing each (geometrical) end point to be placed individually.

The analytical description results in a continuous formulation of the strain energy, derived by Tangential Differential Calculus (TDC) [1-2], with both displacement and rotational degrees of freedom. In conjunction with symbolic automatic differentiation, this facilitates the seamless integration of higher-order approximations and complex geometrically and/or materially nonlinear behaviour.

We discuss the handling of discontinuous geometry and non-standard mesh layouts, followed by numerical tests using the open-source FEM framework, FEniCSx.

[1] A. Sky, J.S. Hale, A. Zilian, S.P.A. Bordas, P. Neff, 2024, Intrinsic mixed-dimensional beam-shell-solid couplings in linear Cosserat continua via tangential differential calculus, Computer Methods in Applied Mechanics and Engineering, https://hdl.handle.net/10993/54222

[2] A. Zilian, M. Habera, 2022, Nonlinear analysis of thin-walled structures based on tangential differential calculus with FEniCSx, https://hdl.handle.net/10993/54222

## S04.05: Structural mechanics

Date: March 18, 2026 16:30–18:30
Room: KI, M11.32
Chair(s): Steinbrecher, Ivo
Sauer, Roger

### Iterative beam fitting with a static mesoscale projection for auxetic lattice structures

Grünfelder, Nicolas; Dieckgraeff, Benjamin; Waschinsky, Navina; Ricken, Tim 16:30
*University of Stuttgart, Institute of Structural Mechanics and Dynamics in Aerospace Engineering*

Auxetic structures form a distinct subgroup of metamaterials and possess unique characteristics, making them of great interest for many engineering applications. Especially noteworthy are the negative geometrical Poisson ratios, high resistance to penetration, and high energy dissipation and absorption capabilities. However, the true advantage of these properties lies in the fact that they are not only inherently beneficial, but result exclusively from the geometric design of the unit cells. This opens up a large design space which offers the opportunity to excel in a wide range of applications. However, this geometric distinctive feature also poses problems for the application of auxetic structures. Because the structures are solely geometry-driven, an accurate resolution of the geometry is essential for calculating the behavior of a structure. This, in combination with the fine geometric mesoscale features in large macroscopic domains, leads to an enormous computational effort.
To solve this problem, a reduced order model using an iterative beam fitting approach is proposed by the authors [1]. This leads to a reduction in the fidelity, while keeping the accuracy close to the high-fidelity solution. The framework models the mesostructured auxetic lattice as Timoshenko beams. However, it can be shown that this beam model leads to inaccuracies in the solution. Consequently, each macroscopic beam is subdivided into sub-spans, with variable cross-section, which are the adjusted by an optimization procedure in order to reduce the error with respect to the high-fidelity solution. The displacement values are extracted for each unit cells in the macroscopic low fidelity simulation and inserted into a high-fidelity simulation of the individual unit cells. A static condensation technique is applied to make this step more efficient, utilizing the periodicity of the grid. The resulting forces are applied to the beam model and the displacement field is recalculated. The deviation between the two beam simulations is incorporated into the optimization as an objective function. Within this contribution a methodology for reducing complex auxetic lattice structures is discussed. Thereby making them usable for simulations or optimizations of entire components and assemblies. This will be further investigated using a number of different examples of auxetic lattice structures, which comprehensively demonstrate the capabilities and restrictions of this approach.
References
[1] N. Grünfelder, et al.(2025), Reduced-order modeling of lattice structures through iterative beam fitting and static mesoscale projection, Results in Engineering, 106529.

### Thermo-Mechanical Optimisation of Dental Implant Drills via Geometrically Optimised Auxetic Mesostructures

Dieckgraeff, Benjamin; Grünfelder, Nicolas; Seyedpour, Seyed Morteza; Ricken, Tim 16:50
*University of Stuttgart, Institute of Structural Mechanics and Dynamics in Aerospace Engineering*

Auxetic structures are a class of additively manufactured metamaterials distinguished by their negative structural Poisson's ratio and, consequently, atypical deformation mechanisms. Components incorporating auxetic mesostructures have also been shown to exhibit negative thermal expansion together with high resistance to penetration and enhanced energy absorption and dissipation. These attributes enable purposeful tuning of structural behaviour primarily through geometry rather than through changes in the base material.

This study investigates whether targeted geometric optimisation of auxetic mesostructures can enhance the macroscopic thermomechanical response of dental implant drills subjected to thermal loading. Thermal effects are clinically relevant, as frictional heat generated during osteotomy may increase local bone temperature, thereby elevating the risk of temperature-dependent necrosis and impairing subsequent healing. Owing to their specific structure, auxetic architectures show a negative thermal expansion and therefore may provide deformation pathways that reduce the local temperature rise under friction-induced thermal loading.

A structured workflow is employed in which the mechanical response is optimised solely by modifying the structural layout and geometry, whilst simultaneously identifying an optimal architecture for the considered load case and drill design. First, a parametric optimisation is carried out to determine favourable geometric descriptors of the auxetic unit cell. These results are then refined using an advanced version of an established shape-optimisation method, enabling region-specific adaptation of mesostructure morphology within the drill macrostructure. The same procedure is applied to a conventional honeycomb mesostructure to isolate and quantify the influence of the auxetic effect. The optimised designs are subsequently compared to identify the configuration offering the most advantageous thermomechanical characteristics, with particular emphasis on minimising local temperature rise.

This work provides new insight into the implementation of optimised auxetic mesostructures and indicates their potential to mitigate friction-induced thermal loading in dental implant drills, thereby supporting improved conditions for bone tissue healing. The results further suggest that auxetic architectures may represent a promising alternative to conventional cellular designs across a range of engineering applications.

**Efficient Beam-Based Simulation of Thermo-Electro-Elastic Lattice Structures**

Alzate Cobo, Juan C.; Nghiem, Xuan Bach; Weeger, Oliver 17:10
*TU Darmstadt*

Lattice structures are widely used as load bearing components in lightweight engineering. However, their full potential lies beyond purely mechanical applications. In comparison to bulk materials, lattices exhibit considerably higher surface-to-volume ratios, which in return directly affects the metamaterial's thermal conductivity. In other words, due to the increased active area and the related increased heat dissipation, lattice metamaterials can build up greater temperature gradients when compared to their bulk counterparts. This characteristic has been recently exploited and lattices have been used as semiconductors in thermoelectric applications. Karthikeyan et al. [1] reported lattice thermoelectric generators (TEGs) with improved mechanical stiffness and a power conversion efficiency of 10%. Note that conventional TEGs have an efficiency of 3% and suffer from severe brittleness. However, since simple FCC lattice structures were reported in [1], the question regarding optimal design remains unanswered.

In this contribution, we present a numerically efficient model capable of accurate thermo-electro-elastic simulations of lattices. The mechanics of the lattice are modeled using the geometrically exact beam theory and the temperature equation is solved by assuming rotational symmetry of the temperature field. The former assumption reduces the 3D continuum mechanics problem to a 1D one and the latter reduces a 3D thermal conduction problem to a 2D one. Hence, numerical efficiency is assured. The solution of the thermomechanical problem is obtained using a staggered solution scheme and the thermoelectric effect is directly obtained from the temperature field in a postprocessing step. Both, the mechanics and the temperature equation, are solved using isogeometric collocation. The model used in this contribution is a direct extension of the beam model introduced by Alzate et al. [2]. Lastly, results are validated against various computationally much more expensive simulations with 3D solid elements conducted in ANSYS.

With this contribution we present a model that replicates the thermo-electro-elastic behavior of TEGs in a way that is both accurate and numerically efficient. Consequently, this model is well suited, yet not limited, for its further use in optimization as well as in homogenization frameworks. The model can also be perfectly used in thermo-elastic applications.

[1] Karthikeyan, V., Surjadi, J.U., Li, X. et al. Three dimensional architected thermoelectric devices with high toughness and power conversion efficiency, Nat Commun 14, 2023.

[2] J. C. Alzate Cobo, X.-L. Peng, B.-X. Xu, and O. Weeger. A finite swelling 3D beam model with axial and radial diffusion, Comput. Methods Appl. Mech. Eng., 441, 2025.

**Investigation of Geometrically and Materially Induced Artificial Instabilities in Mixed Nonlinear Finite Element Formulations**

Jakob, Henrik; Bischoff, Manfred 17:30
*Universität Stuttgart, Germany*

For geometrically linear problems, locking behavior is a well-researched field and may be considered as mostly, though not fully, solved. However, for geometrically nonlinear finite element formulations, new problems arise when using locking-free formulations. For this contribution we will focus mainly on finite elements that use an enhanced assumed strain (EAS) field to overcome locking effects.

One pronounced problem in EAS elements and similar methods is the occurrence of artificial instabilities in the form of hourglassing for large deformations (cf. Armero (2000)). For compression problems, instabilities induced by the geometric stiffness can lead to a buckling phenomenon, akin to the well-known Euler-buckling, on element level. This effect is henceforth called geometric hourglassing. Finite element formulations that cure these effects by modifying the Green-Lagrange strain were recently proposed by Bieber et.al (2023).

On the other hand, for the tensile case, a similar effect can be observed. Here instabilities emanating from the material stiffness trigger hourglassing. This effect can be linked to instabilities in the used material law; therefore, we call it material hourglassing. A prominent example is the strain-softening effect found in elastoplastic material behavior. Also, certain hyperelastic material laws behave similarly and can lead to hourglassing.

This contribution aims to develop finite element formulations that do not suffer from these artificial instabilities. We propose the following criteria, that novel formulations should adhere to: firstly, being free from all linear and nonlinear locking behavior, secondly, being free from artificial instabilities but still being able to capture physical instabilities, and lastly, the formulations have to be independent of the used material law and integration scheme.

To achieve this, we will first investigate the causes and effects of material instabilities both in the material law and the EAS element formulations. Next, finite element formulations that treat the occurrence of hourglassing using a similar approach to the aforementioned contribution by Bieber et.al are investigated.

**Tubular interlockings with internal and external sinusoidal shaping: geometric influence on performance**

Weiß, Meike (1); Macek, Domen (2); Akpanya, Reymond (3); Brepols, Tim (2); Holthusen, Hagen (4); Niemeyer, Alice C. (1) 17:50
*1: Chair of Algebra and Representation Theory, RWTH Aachen, Germany*
*2: Institute of Applied Mechanics, RWTH Aachen University, Germany*
*3: The School of Mathematics and Statistics, The University of Sydney, Australia*
*4: Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

Topological interlocking assemblies (TIA) are arrangements of blocks kinematically constrained by a fixed frame, such that all rigid body motions of the blocks are prevented by the neighbouring blocks and the frame. In our previous papers [1, 2] we have verified that the design and the arrangement of the blocks indeed have an influence on a planar TIAs' mechanical performance. In this work, we examine the influence of design and arrangement for tubular TIAs (blocks arranged in a tubular structure) motivated by building mortarless pillars. Inspired by the sine-curve, we present a new block depending on one parameter. The parameter describes whether the outer or the inner surface of the tube is deformed to construct curved blocks with sinusoidal shapes on the deformed surface. We investigate the influence of this design parameter on the mechanical performance of the resulting TIA. First, we employ a simplified multi-body dynamics approach that enables rapid evaluations

of how the position of the sinusoidal shape influences load transfer within the assembly. We then examine several boundary-value problems representative of tubular structures—for example, pillar- and beam-like configurations. Furthermore, we validate our findings by conducting FEM simulations which additionally give insights into the mechanical behaviour (deformation, peak stresses) of the TIA. Our results show that the position of the sinusoidal deformation has an influence on the structural performance of the TIA. Based on our results we characterise suitable blocks for prescribed boundary value problems.

References

[1] T. Goertzen, D. Macek, L. Schnelle, M. Weiß, S. Reese, H. Holthusen, and A. C. Niemeyer. Influence of block arrangement on mechanical performance in topological interlocking assemblies: A study of the versatile block. International Journal of Solids and Structures, 306:113102, 2025.

[2] L. Schnelle, M. Weiß, R. Akpanya, K.-U. Schröder, and A. C. Niemeyer. Influence of a generative parameter on the mechanical performance of topological interlocking assemblies of a hexagonal block. arXiv:2512.03941. Accepted for publication at CIRP Design, 2026; Tokyo, Japan.

**Investigation of forming forces and energy dissipation rate in steady-state elastic-plastic bending of an axially moving beam**

Ramsauer, Stefan; Scheidl, Jakob
*TU Wien, Austria*

18:10

In continuous metal forming, material is transported without interruption through a series of forming stands that sequentially induce plastic deformations to achieve a certain forming goal. A steady supply of mechanical energy is required to sustain the process and counterbalance energy dissipation due to plastic forming. If the contact of the moving material with the forming tools is assumed to be frictionless, active forces at the boundaries of the mechanical model must supply the necessary power. The identification of the power balance including the quantification of these forces is inherently difficult to achieve with conventional Lagrangian models, where the mechanical model contains a fixed material volume, whose boundaries are transported with the material particles along the forming line. A mixed Eulerian–Lagrangian model with fixed spatial domain allows for a full analysis by taking into account the interaction with the resting tools and the boundary conditions at the spatially fixed boundaries, where material particles are continouosly entering and leaving the control domain.

Here, we adopt such a Eulerian parametrisation to study the elastic-plastic bending of an axially moving Euler–Bernoulli beam. In this comparatively simple mechanical model, kinematic transverse loading mimics the frictionless contact with the forming tools and induces elastic-plastic deformations. Elasto-plasticity is resolved with a structural plasticity model for pure bending of an elastic ideal-plastic cross-section.

The conditions of stationary forming operation are utilized to obtain semi-analytic solutions of the geometrically linear problem. These analytic reference results are used to address the mechanical power balance as well as the validation of a novel finite element model. The latter features a stationary predictor-corrector method that takes the conditions of stationary operation into account when iteratively seeking a quasistatic elastic-plastic equilibrium. This augmented algorithm directly yields a stationary state for each load increment, which makes it more efficient and better-suited for parameter studies than conventional time-driven procedures. Furthermore, this numerical model allows for a convenient analysis of the interaction forces and the work they produce.

## S04.06: Structural mechanics

Date: March 19, 2026 08:30–10:30
Room: KI, M11.32
Chair(s): Neu, Gerrit Emanuel
Altay, Okyay

**A Variational Physics-Informed Neural Network Framework for Simulating Nonlinear Elastic Wave Propagation**

Ankay, Benjamin; Altay, Okyay 08:30
*Chair of Structural Analysis, Department of Civil Engineering, University of Siegen, Germany*

This work adopts Variational Physics-Informed Neural Networks (VPINNs) to address the forward problem of wave propagation in two-dimensional nonlinear elastic solids. A first-order formulation of the elastodynamic governing equations is employed, in which particle velocities and strains constitute the dependent field variables. Furthermore, a specific variant of the VPINN approach is used, in which the residuals are constructed elementwise. This formulation — commonly referred to in the literature as an hp-VPINN — enables the direct transfer of finite element concepts, such as local approximation spaces, numerical quadrature, and domain decomposition, into the VPINN framework. Within this hp-VPINN structure, the first-order formulation ensures that all required spatial and temporal derivatives appear exclusively in weak form. Consequently, the evaluation of the residuals relies solely on first-order gradients, which can be computed directly during training without automatic differentiation of higher-order derivatives. This improves numerical efficiency and stability, which is particularly important for wave-propagation problems where strong nonlinearities or steep gradients often lead to differentiation-induced errors. Moreover, VPINNs naturally accommodate absorbing boundary conditions without mesh generation or specialized boundary treatments, making them well suited for large-scale or geometrically irregular domains.

The present work investigates the feasibility of the proposed framework in a nonlinear elastic medium, with a focus on stability, accuracy, and boundary-condition enforcement. Particular attention is given to the formulation of nonlinear constitutive relations, the handling of coupled field variables, and the weak enforcement of the governing equations through appropriate test functions and quadrature rules. The study evaluates the ability of the VPINN framework to reproduce characteristic features of nonlinear wave propagation, such as harmonic generation and waveform distortion, and examines its sensitivity to parameter variations. Overall, the results demonstrate that VPINNs provide a powerful and flexible alternative to classical PINNs for forward modeling of nonlinear ultrasonic waves, while simultaneously establishing a solid basis for future inverse methods aimed at extracting nonlinear material parameters from wavefields, with a particular focus on applications in damage detection and structural health monitoring (SHM).

**Oscillatory Physics-Informed Neural Networks (oPINN) for vibrating continua**

Hildebrand, Stefan; Klinge, Sandra 08:50
*Technische Universität Berlin, Germany*

Thanks to their high versatility, Physics-Informed Neural Networks (PINN) methods [1] have been

successfully applied to a broad variety of problems in elastostatics, heat transfer, material modeling and fluid flow [2 - 4]. For the application of vibrating continua, where conventional PINNs show poor convergence, oscillatory Physics-Informed Neural Networks (oPINN) are proposed. They allow for a great variety of hybrid Physics-Informed and data-driven analyses of structures. Among others, sparse or noisy vibration measurements can be integrated with structural modeling to

obtain an accurate and comprehensive system representation. Moreover, estimates of a structure's eigenfrequencies of linear systems can be included as an input to reduce the computational effort. As an important advantage, Dahlquist's barriers [5] are circumvented since no conventional time-stepping scheme is applied. The validation of the suggested approach is carried out by comparison with a conventional Adams Predictor-Corrector time integration scheme. The results show that the oPINN approach achieves accuracy comparable to the conventional time integration schemes. High stability, especially in numerically challenging cases is demonstrated as well. Finally, it has been demonstrated that Curriculum Learning can significantly enhance computational efficiency for series of similar setups, which are common in parameter studies, optimization of structures and multi-frequency excitation analyses.

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**Characterization of a foundation slab for reuse by inverse identification methods**

Neuhaus, Neil (1); Qaddoura, Mohamad Sami (2); Trapp, Maximilian (2); Knorr, Peter (3); Nestorović, Tamara (2); Wichtmann, Torsten (3); König, Diethard (3); Hackl, Klaus (1); Waimann, Johanna (1)

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*3: Chair of Soil Mechanics, Foundation Engineering and Environmental Engineering, Universitätsstraße 150, 44801 Bochum, Germany*

09:10

Concrete is one of the world's most important building materials. However, its production is very resource-intensive. Reusing existing structures could be a step towards greater sustainability, a possibility that is being investigated in the Collaborative Research Center 1683. We would like to present initial results dealing with the characterization of a foundation slab and the soil below. A basic prerequisite for the reuse of the slab after demolition of the original structure is that the structure is in sufficient condition. The aim of subproject B04 is to characterize the remaining material properties and residual load-bearing capacity using inverse calculation methods. Some examples for the application of such methods to elastic boundary value problems are [1] and [2]. The inverse methodology to be developed will be based on measurement data on the mechanical loading as well as on the uplift of the foundation at various positions and steps during the deconstruction process.

As the deformations are usually small, Kirchhoff Love plate theory in combination with the finite difference method is used to describe the foundation slab. In a first step, the slab's stiffness is assumed to be constant. Following [3], a Winkler foundation is assumed, and the soil is thus represented by linear springs. Using an inverse optimization scheme, the stiffness of the springs can be detected which fits to the measured data for the loads and resulting displacements. We will show the method's performance based on artificial data as well as its validation using experimental data stemming from small-scale laboratory experiments as well as real-scale field measurements.

References:

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**Reducing Overestimation in Interval-Based Frequency Domain Analysis of Structures with Viscoelastic Dampers under Parameter Uncertainty**

Łasecka-Plura, Magdalena 09:30
*Poznan University of Technology, Poland*

Accounting for uncertainties in design parameters is one of the key challenges in modern analysis of civil engineering structures and mechanical systems. Uncertainties may arise from an inaccurate representation of material properties, geometry, boundary conditions, or loads. In dynamic problems, they can significantly affect the structural response, and neglecting them may lead to substantial errors in assessing the system behavior.

Methods for uncertainty quantification can be divided into probabilistic and non-probabilistic approaches. Probabilistic methods, although widely used, require identification of probability distributions of random variables, which is not always feasible. Non-probabilistic methods, in turn, can be used to estimate only the range of system responses, which is often sufficient from an engineering perspective. Interval analysis is particularly useful in this context and can be applied to viscoelastic elements, for which determining parameter distributions is very difficult. It enables the computation of lower and upper bounds of the structural response.

In practice, however, applying interval analysis to dynamic problems is associated with significant overestimation, arising, among others, from multiple occurrences of the same interval variables and from the loss of correlations between variables during matrix operations. This may result in excessively wide response intervals, making the results of limited usefulness for engineering purposes. Therefore, reducing overestimation is essential for obtaining reliable results.

This contribution presents an approach for determining the frequency response functions (FRFs) of a shear frame with viscoelastic dampers. Both classical and fractional rheological models are considered. The equations of motion, formulated in the frequency domain, are transformed into a linear system of equations from which the FRF components can be obtained. A key element of the proposed approach is transforming the derived equations so that each interval quantity associated with a given uncertain parameter appears only once in the formulation, combined with an element-by-element representation. This allows the resulting FRF envelopes to be narrower compared with direct interval arithmetic.

The obtained results will be compared with the vertex method and with an iterative approach based on fixed-point iteration method. For fractional models, uncertainty in the fractional derivative order will also be taken into account, for which a hybrid strategy is considered.

**Identification of Updated Voce-Chaboche Constitutive Model Parameters Using Convolutional Neural Networks**

Zhang, Bingzhe (1); Lignos, Dimitrios (2); Altay, Okyay (1) 09:50
*1: Chair of Structural Analysis, Department of Civil Engineering, University of Siegen, Germany*
*2: Resilient Steel Structures Laboratory, School of Architecture, Civil and Environmental Engineering, École Polytechnique Fédérale de Lausanne, Switzerland*

This study presents a data-driven framework for identifying parameters of the Updated Voce–Chaboche (UVC) constitutive model commonly used for simulating the inelastic behavior of structural steels. The approach exploits uniaxial stress–strain responses of specimens subjected to ten representative strain-controlled loading protocols, including standardized monotonic, cyclic, and increasing-amplitude histories. An autoencoder-type architecture is adopted, consisting of coupled inverse and forward convolutional neural networks (CNNs). The inverse model maps measured stress responses to UVC parameters, whereas the forward model maps parameters back to stress histories. Their composition yields a stress-to-stress mapping that regularizes the inverse problem and mitigates the typical ill-posedness of parameter identification.

First, the forward model is trained on synthetic stress responses generated by the UVC model for Latin hypercube–sampled parameter sets within physically admissible ranges; stresses are evaluated at selected strain levels for all ten loading protocols. To improve generalization and reduce overfitting, controlled noise is introduced during training to emulate practical uncertainties. With the forward model frozen, the inverse model is subsequently trained by feeding synthetic stress responses and minimizing the discrepancy between reconstructed and original stress histories, thereby enforcing forward–inverse consistency. After training, the inverse model directly estimates UVC parameters for new specimens from measured stress responses under the same loading protocols.

The proposed approach is evaluated using physical data from test specimens extracted from 24 different hot-rolled steel profiles and plates. All specimens were previously tested under the ten prescribed loading protocols, and the resulting stress responses are used to identify UVC parameters via the trained inverse network. The identified parameters and reconstructed stress responses are benchmarked against a classical gradient-based optimization approach using algorithmic differentiation, in terms of computation time and hysteresis-loop area of the stress–strain response. On a workstation equipped with a 24-core CPU, 64 GB RAM, and a 20 GB GPU running Linux, the proposed method completes data generation, training, and parameter identification for all specimens in approximately 15 minutes, whereas the classical approach requires nearly 15 hours, demonstrating a substantial reduction in computational cost. Once trained, the network identifies parameters for additional specimens within milliseconds without retraining, whereas gradient-based optimization requires more than 30 minutes per specimen. On average, the proposed CNN-based framework attains a mean relative error of 6.9%, close to the 6.2% achieved by the classical approach. These results indicate that the proposed framework provides a fast yet robust tool for UVC parameter identification.

**Effect of internal structures on particle damper performance: Assessing the predictive capability of LIGGGHTS open source Discrete Element Method (DEM) modeling tool**

Lokhande, Harshad; de Payrebrune, Kristin M. 10:10
*RPTU Kaiserslautern-Landau, Germany*

Particle dampers are non-linear, passive energy dissipation devices designed to be mounted on or embedded within a vibrating structure to effectively reduce its amplitude. These dampers consist of an enclosed cavity containing granular media, typically particles composed of materials such as steel, glass, lead, soda lime glass or sand [1][2]. The damping mechanism involves the dissipation of the structure's kinetic energy into heat, primarily by repeated inelastic inter-particle and particle-wall collisions and frictional losses. Despite their promise, widespread adoption is limited by the inherent complexities and non-linearity of performance. Critically, their behavior is dependent on several parameters such as fill ratio, vibration amplitude, and frequency, which complicates optimal design and predictive understanding.

To address the challenges of modeling their nonlinear behavior, this research presents an investigation focused on quantifying the performance of various particle damper cell designs with internal structures in the form of barriers. Experimental analysis was conducted to determine the loss factor of various particle damper, calculated using a complex energy formulation [3]. The results of standard particle damper cells were compared against those designed with internal barrier structures. Furthermore, the physical experiments were computationally simulated using the Discrete Element Method (DEM) formulation within the open-source software *LIGGGHTS* [4]. This allows for an independent calculation of the loss factor from the DEM simulation data, which was compared with the empirical output.

The crucial comparison highlights both the predictive limitations and general capability of the *LIGGGHTS* DEM simulation software for accurately modeling the performance and for designing effective particle dampers.

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## S04.07: Structural mechanics

Date: March 19, 2026 14:00–16:00
Room: KI, M11.32
Chair(s): Gudžulić, Vladislav
Klarmann, Simon

### Simulation of crack initiation in a heterogeneous domain

Medda, Ronjit; Müller, Ralf 14:00
*Technical University Darmstadt, Germany*

Steel rolling bearings, which are widely used e.g. in wind turbines, have been found to fail prematurely as a result of two distinct fracture related phenomena labeled 'white etching cracks' (WEC) and 'fine-granular area' (FGA)[1], respectively. Possible common mechanisms in the formation of both failure types are currently being investigated in a joint research project (DFG FOR 5701), involving both experimental and simulative approaches.

Focusing on the observed interaction between WECs / FGAs and inclusions[2], this presentation provides an overview of the numerical simulation of the mechanical fields in the vicinity of inclusions in a 100Cr6 steel matrix, especially with regard to fracture-inducing stress concentrations.

The chosen numerical setup combines a finite element discretization of a heterogeneous domain (matrix + inclusion) with a fracture phasefield[3] on the assumption of isotropic material behaviour, quasi-static conditions and geometrically linearized strains.

In order to capture the plastic hardening capacity of steel, a Ramberg-Osgood-type physically nonlinear stress-strain relation is employed for the matrix material, while the typically stiffer inclusions are modeled with linear-elastic behaviour.

It will be shown that this modeling approach is capable of predicting different loci of stress concentration and accordingly, crack initiation, depending on the material properties of the inclusions.

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**An AceGen Interface for the Efficient Analysis of Gradient Damage Problems in Ferrite.jl**

Geht, Artur; Miska, Niklas; Balzani, Daniel 14:20
*Chair of Continuum Mechanics, Germany*

Since local damage formulations suffer from mesh-dependency and loss of ellipticity, regularizations such as gradient enhanced formulations can be used to recover mesh-independency and numerical robustness. As these approaches often require mixed finite elements, in which a damage variable is considered as primary variable in addition to the displacement field, intricate derivatives are required, which is why finite element code generators capable of automatic differentiation such as e.g., AceGen on top of Mathematica, are advantageous. While AceGen provides bindings and interface to proprietary finite element codes such as AceFem, Feap or Abaqus, it may be beneficial to couple the generated elements with open source finite element codes such as Ferrite.jl, which is a finite element toolbox implemented in the emerging programming language Julia. In this contribution, the development of an interface between an AceGen-generated mixed finite element for gradient damage in the programming language C and the Ferrite.jl toolbox is presented. Key points are the discussion of arising hurdles, when different programming languages and finite element codes are coupled, such as e.g., the differing memory layout of variables, the concept of memory pointers as well as different node orderings within the finite element and tensor representations. For this purpose, a nested software module will be presented, which addresses the appropriate processing of variables and their format, calling of the element in a different language, recasting of the stiffness matrix and residual vector for use in the finite element context of Ferrite.jl as well as a static condensation to ensure efficiency and robustness of the finite element simulation.

**Pressure-Induced Deformation in curved and fiber-reinforced flexible hoses: From 3D continuum simulation to experiments**

Hoesch, Quirin (1,2); Roller, Michael (1); Schneider-Jung, Fabio (1); Linn, Joachim (1); Müller, Ralf (2) 14:40
*1: Fraunhofer Institue for Industrial Mathematics ITWM, Germany*
*2: Technical University of Darmstadt, Germany*

The virtual safeguarding of vehicle cables and hoses requires a digital simulation tool that is both computationally efficient—enabling realtime performance—and physically reliable. Although geometrically exact rod formulations have proven effective for modeling highly flexible slender structures, their predictive capability for deformations is limited when applied to curved, pressurized hoses with anisotropic material behavior resulting from the embedded fiber reinforcements.

We therefore analytically investigate the dominant effects governing the mechanical response of curved hose segments that can be conceptualized as toroidal components. A key aspect is the coupling between curvature and internal pressure, which generates a curvature-dependent outward shear force on the macroscale—the Bourdon effect—and additionally exhibits characteristic cross-sectional deformations on the mesoscale, due to the inherently coupled axial-radial response of the closed ring toroidal structure. Moreover, we analyze the interaction between curvature and the reinforcing helical fibers, as the double-curved toroidal surface induces a variation of the fiber wrapping angle along the cross-section. Finally, we examine the coupling between internal pressure and the helical reinforcements, showing that the toroidal neutral wrapping angle establishes an isotensoidal stress state by balancing axial and circumferential stresses and aligning the fibers along the principal stress resultant.

The analytical predicitons are subsequently validated using highly resolved 3D continuum finite element models and suitable homogenization approaches for the fiber reinforcements. The predicted deformation patterns are validated by hose-test-rig experiments supported by CT-based fiber-structure characterization. Despite unknown material parameters, sensitivity-based parameter identification enables accurate simulation agreement with the experimental deformation patterns. These

combined analytical, numerical and experimental insights are intended to identify relevant deformation mechanisms and to evaluate their transferability to a reduced-order shell or beam formulation suitable for real-time simulations.

**Viscoelastic Constitutive Modelling for Cable Simulation: A Computational & Experimental Assessment**

Shirke, Atharva (1,2); Schneider-Jung, Fabio (1); Linn, Joachim (1); Weeger, Oliver (2) 15:00

*1: Fraunhofer Institute for Industrial Mathematics (ITWM), Fraunhofer Platz 1, 67663 Kaiserslautern, Germany*
*2: Cyber-Physical Simulation, Department of Mechanical Engineering, Technical University of Darmstadt, Dolivostr. 15, 64293 Darmstadt, Germany*

Flexible slender structures such as cables, hoses, and robotic umbilicals are becoming increasingly central to modern engineering systems, particularly in electric vehicles, autonomous platforms, and high-performance robotics. Their dynamics are dominated by large deformations and frequency-dependent dissipation mechanisms that are captured by viscoelastic models within simulation. The geometrically exact Cosserat rod theory has emerged as an efficient framework for modelling such systems, mainly due to its low computational cost and its ability to represent extensional, shear, bending, and torsional deformations.

Despite the strength of the Cosserat formulation in capturing geometrically nonlinear dynamics, its constitutive modelling typically relies on the Kelvin–Voigt (KV) model, which is a linear viscoelastic law. To investigate frequency-dependent damping behavior experimentally, we excite the cable using constant, linear and quadratic frequency chirps, which sweep through a wide range of frequencies and reveal how dissipation evolves across the spectrum. KV can be tuned to match measured responses within a limited excitation band; however, as the frequency band broadens—as it does under chirp excitation—its single relaxation timescale becomes insufficient, leading to systematic errors in the simulations.

To address these limitations, we introduce a multi-branch Generalized Maxwell (GM) constitutive model into the Cosserat framework, enabling a multi-timescale and frequency-responsive description of viscoelasticity without altering the underlying rod kinematics. By representing the material as a combination of parallel Maxwell branches, the GM formulation captures multiple relaxation processes simultaneously, allowing it to reflect how real materials dissipate energy differently across low, mid, and high frequencies. This multi-timescale structure provides the flexibility needed to simulate broadband damping behavior.

Comparisons between simulated and measured responses, based on the parameters obtained via optimization against experimental data, show that the GM-based model consistently exhibits closer alignment with observed behavior than the KV law. Although the multi-branch structure introduces additional complexity in parameter identification, the resulting improvement in predictive fidelity is substantial.

Overall, the results verify that the GM model for viscoelasticity provides the accuracy required for broadband dynamic modelling, exceeding the capabilities of KV. Moreover, emerging data-driven approaches—including machine-learning based parameter identification—are worth exploring as potential next steps for enhanced constitutive modelling of the nonlinear modelling behavior of flexible slender structures.

**Displacement-Based Multiaxial Cycle Counting for the Progressive Damage Analysis of a Wind Turbine Blade**

Fink, Richard; Häusler, Stephan; Radtke, Lars; Sander, Manuela 15:20

*University of Rostock, Germany*

The structural integrity of wind turbine blades depends critically on accurate predictions of the stiffness degradation under complex, multiaxial loading. Traditional fatigue assessments often rely on uniaxial rainflow counting coupled with a linear damage accumulation. However, these approaches

fail to capture the progressive stiffness reduction inherent to composite materials under multiaxial loading.

Conventional multiaxial counting methods such as critical plane and average stress theories, require a known stress history. However, in the presence of stiffness degradation, the stress state evolves continuously, creating an implicit dependency on the cycle count that renders these stress-based methods invalid. This study adresses alternative displacement-based projection methods, specifically random hypersphere sampling and singular value decomposition, using synthetic time history of the blade deformation data resulting from beam simulations of a stochastic wind field.

The resulting cycle blocks are applied to a 3D shell model of a state-of-the-art blade. Unlike standard fatigue life predictions, this framework combines the counting outputs directly with a progressive damage model to account for the non-linear evolution of damage. The analysis focuses on the correlation between the chosen counting method and the stiffness degradation of critical sections. The study demonstrates that counting strategies based on projections yield distinct degradation paths compared to simple component-wise decomposition methods. This highlights the necessity of decoupling cycle counting from the stress evolution in composite fatigue analysis.
This study was supported by the German Federal Ministry for Economic Affairs and Climate Action, 11019 Berlin (Funding number: 03EE2058C)

**Experimental Validation of a Static Digital Twin for Reducing the Formwork Support Time of Reinforced Concrete Ceilings**

Müllner, Herbert W. (1); Posch, Raphael E. (2); Harrer, Johannes A. (3); Rauch, Christian (1)
*1: PORR Bau GmbH, Technology Management and Innovation, Austria*
*2: PORR Bau GmbH, Building Construction, Austria*
*3: Harrer & Harrer ZT-GmbH, Austria*

15:40

The structural design of reinforced concrete ceilings is mainly based on finite element calculations. Increasingly tighter construction schedules and cost pressures on construction sites ultimately lead to situations where the shoring periods specified in the structural analysis can no longer be met. After early formwork removal, temporary shoring is typically installed on site to comply with the required support duration of the ceilings. This common practice, however, is not examined within the framework of the structural analysis of the ceilings. In addition, climatic conditions and construction phases are also not considered in the calculations. This results in difficulties in meeting the deformation limits prescribed by the standards.

To investigate real ceiling deformations, a research project was carried out in cooperation between the University of Applied Sciences Campus Vienna and PORR Bau GmbH [1]. For this purpose, deformation measurements of the concrete ceilings were carried out during the construction of a residential building complex in Vienna's 3rd district from the ground floor until completion of the structural shell.

In this contribution the empirically determined load approach [2] for finite element calculations will be applied to a 3D model for the detailed structural analysis. To examine different shoring durations of the ceilings, partial models are created depending on the construction stage of the structural shell, considering the temporary shoring present at each stage. For the respective construction stages, on-site measurements from multiple floor slabs are collected, providing a basis for validating the structural sub-models and determining the actual stiffness conditions in the structural shell. This applies not only to ceiling stiffness, but also to wall stiffness and the wall connections of the floor ceilings in the 3D model. For this validation, over 500 simulations were performed for different construction stages with different combinations of stiffness ratios.

Furthermore, the research project aims to help prevent damage and optimize construction processes as well as the time required for subsequent finishing work.

[1] R.E. Posch: Experimental Validation of a Static Digital Twin for Reducing the Formwork Support Time of Reinforced Concrete Ceilings, Master Thesis, University of Applied Sciences, 2026, in German.

[2] H.W. Müllner, S. Filipas, C. Rauch: Experimental Determination of a Load Approach FE-Method for Reducing the Formwork Support Time of Reinforced Concrete Ceilings; PAMM, 25 (2025), https://doi.org/10.1002/pamm.70018.

## S04.08: Structural mechanics

Date: March 19, 2026 17:30–18:30
Room: KI, M11.32
Chair(s): Sauer, Roger
Neu, Gerrit Emanuel

### A Computational Multiscale Framework for Shakedown Analysis of Particle-Reinforced Metal Matrix Composites(PRMMCs)

Veludandi, Lavakumar; Vafadari, Reza; Ochoa, Lilian Aurora; Simon, Jaan Willem 17:30
*University of Wuppertal, Germany*

Particle Reinforced Metal Matrix Composites (PRMMCs) are increasingly used in the aerospace and automotive industries because of their high strength-to-weight ratio and superior wear resistance. However, their long-term structural performance under cyclic and variable loads remains largely unexplored, particularly in safety-critical applications where failure must be prevented over extended service life.

Shakedown analysis, in particular Melan's static theorem, offers a promising approach to assess the long-term behavior of structures under variable loading conditions. Despite its potential, its application to PRMMCs has remained limited, as traditional modeling approaches often idealize the microstructure and overlook the intrinsic heterogeneity of these composites, failing to capture critical local interactions between reinforcement particles and the matrix. Recent investigations, such as those of Chen et al., have started to address these limitations by incorporating micro-structural characteristics and boundary effects, thus laying the groundwork for a more accurate shakedown assessment of PRMMC-based structural components.

This work proposed a multiscale computational framework for lower-bound shakedown analysis of PRMMCs, building upon the methodology of Simon et al., which was originally formulated on the basis of Melan's theorem. Realistic yet synthetic 3D micro-structures were generated, accurately capturing particle morphology, size, and spatial distribution. Homogenization techniques were then applied to extract effective material properties from Representative Volume Elements (RVEs), which were subsequently used in macroscopic shakedown analysis. The methodology enabled investigation of the influence of micro-structural features such as particle size, volume fraction, and boundary conditions on shakedown limits.

By bridging realistic micro-structural modeling with lower-bound shakedown theory, this framework provided a reliable and computationally efficient tool for assessing PRMMCs performance under complex loading conditions. The results demonstrated the effectiveness of the framework in conducting shakedown analysis, predicting shakedown limits, and supporting the safe, optimized design of next-generation lightweight structural components and materials for high-performance structural applications.

### Geometry-informed surrogate modeling for architected metamaterial design under high-rate loading

Gärtner, Til (1); Wang, Haoning (1); van den Boom, Sanne J. (3,4); Sluys, L. J. (2); Aldakheel, Fadi (1) 17:50
*1: Institute for Mechanics and Computational Mechanics, Leibniz University Hannover, Germany*
*2: Faculty of Civil Engineering and Geosciences, Delft University of Technology, The Netherlands*
*3: Netherlands Institute for Applied Scientific Research (TNO), The Netherlands*
*4: Faculty of Mechanical Engineering, Delft University of Technology, The Netherlands*

In recent years, a significant focus of research has been on architected materials, including mechanical metamaterials. The increased prevalence of additive manufacturing technologies and generative design methodologies has led to demonstrable industrial relevance in a wide range of applications,

including medical implants, sports equipment, and ballistic protection. The latter inherently results in large deformations at high rates, including nonlinearities and contact, which renders the prediction of the resulting mechanical responses a challenging task. This is particularly demanding due to the complex interplay between static instabilities and dynamic localization in inelastic materials [1]. While earlier studies have examined the connection between local instabilities and the macroscopic behavior based on the design of individual unit cells [2], the dynamic behavior of larger patches remains to be elucidated.

The design of mechanical metamaterials for high-rate applications requires a focus on the dynamic response of the structure. Computational tools facilitate the investigation of the detailed structural response of architected metamaterials across various spatial scales, which is not possible with experimental investigations. A more profound comprehension of the behavior of structured materials under high strain rates is enabled by the investigation of collapse patterns in singular unit cells as well as larger patches across different strain rates using beam-based finite element investigations. For identification of promising material configurations, computationally less expensive surrogate models are needed to allow for targeted use of the high-fidelity models. The consideration of geometric information based on the design of the unit cell enables calibration of these surrogate models with a reduced dataset.

In this investigation, the effects of changes in the design of a unit cell on the response of macroscopic patches are investigated. The use of structural finite elements together with a machine learning framework informed on geometric aspects of the structure facilitates the investigation of a diverse array of designs and loading conditions.

[1] Gärtner et al. (Dec. 2025). Mater. Today Adv. 28.

[2] Zhang et al. (Apr. 2025). Adv. Mater. 37.

**Automatic Model Identification and Calibration of Hyperelastic Materials based on Digital Image Correlation and Bayesian Inference**

Nguyen, Duc Hoang; Weißenfels, Christian 18:10
*Universität Augsburg, Germany*

The continuous development of increasingly complex engineering materials necessitates advanced modeling strategies that enable reliable optimization of performance and cost already during the virtual design phase. Achieving this objective requires accurate predictive models and an improved epistemic understanding of the underlying material behavior. Additionally, substantial advances in experimental characterization techniques and data-driven methodologies have led to the availability of rich, high-dimensional datasets. While machine learning methods offer powerful tools for extracting patterns from such data, purely black-box approaches often suffer from limited physical interpretability and reduced generalizability. Consequently, there is a growing demand for data-driven frameworks that combine predictive capability with physical transparency.
In this work, a novel data-driven methodology for the identification of constitutive laws governing isotropic hyperelastic materials is presented. The approach integrates sparse regression techniques with Bayesian inference to identify compact and physically interpretable functional representations of the strain energy density. Starting from a comprehensive library of candidate functions based on commonly used strain invariants and nonlinear measures, the method systematically selects only terms that are essential for accurately describing the observed material response. This yields parsimonious constitutive models that retain clear physical meaning and can be seamlessly incorporated into established FEA frameworks.
The methodology exploits full-field displacement data obtained from experimental measurements, for instance by means of DIC, which provide spatially resolved information on the deformation state. By leveraging such data, the approach goes beyond traditional calibration strategies based on global stress-strain responses and enables the identification of material behavior under heterogeneous deformatios. To account for measurement noise, modeling uncertainties, and potential simplifications in the assumed constitutive structure, global and local regularization strategies are embedded within a Bayesian probabilistic framework. This formulation naturally enables uncertainty quantification,

allowing the confidence in both the identified constitutive structure and the estimated material parameters to be rigorously assessed.
A key component of the proposed framework is the calibration of the identified constitutive models through an inverse analysis procedure. For this, experimentally measured displacement fields are directly coupled with displacement fields obtained from FEA based on the candidate material models. Model parameters are iteratively updated by minimizing discrepancies between simulated and observed displacement fields within a Bayesian inference setting. This inverse approach yields not only optimal parameter estimates but also posterior distributions that explicitly quantify uncertainties arising from experimental imperfections and modeling assumptions. The capabilities and robustness of the proposed methodology are demonstrated using synthetic benchmark examples representing a range of isotropic hyperelastic behavior.

## S04.09: Structural mechanics

Date: March 20, 2026 08:30–10:30
Room: KI, M11.32
Chair(s): Klarmann, Simon
Gudžulić, Vladislav

### Accuracy analyses on test strain determination for the calibration of strain gages

Lehmann, Thomas; Jähnichen, Tobias; Ihlemann, Jörn 08:30
*Chemnitz University of Technology, Germany*

In experimental solid mechanics, strain is a very frequently determined quantity. Strain measurement methods are available with different characteristics, e. g., in terms of operating principle, strain measurement range and analysis region (point or field measurement methods). Classic electrical strain gages are still very relevant in their application today due to outstanding precision and accuracy. The requirements for calibrating strain gages, and in particular the associated determination of test strain, are high.

In this contribution, accuracy analyses with regard to test strain during the calibration of strain gages are presented. A four-point bending setup with aluminum specimen is used. This load case is suitable for this purpose due to the clearly defined deformation conditions in the examined section of the specimen. Strain gages are applied between the load application sections. The specimen is loaded up to a maximum force that results in small strains within the elastic range of the metal. Two different measurement methods for determining test strain are tested in terms of their achievable accuracy: the use of incremental displacement transducers (as contact measuring system) and 3D digital image correlation (DIC). When using displacement transducers, the test strain determination is based on deflection differences, which are detected at the bottom of the specimen. Ideal pure bending results in a constant curvature (at the respective position of the beam cross-section in loading direction, circular arc). With the DIC variant, the raw displacement data in transverse direction (loading direction) on the front surface of the specimen is approximated by a circular arc fit. The test strain is calculated by means of the resulting curvature radius. Furthermore, the gage factor is obtained using the respective test strain and the Wheatstone bridge output of the strain gage. The two different methods show good agreement of the determined test strain with high accuracy. This is also demonstrated by small relative deviations (for higher loads) of the gage factor from the data sheet value of the strain gages using both methods. In particular, it has been proven that the evaluation method used allows the DIC measurement range to be extended to smaller deformations. Due to contact with the specimen, the accuracy of the displacement transducer method is limited in repeated measurements when surface defects occur.

**Observing Modal Coordinates with Integrated Motion Measurement Systems for Structural Health Monitoring**

Kohl, Michael; Wagner, Jörg F. 08:50
*Chair of Flight Measuring Technology, University of Stuttgart, Germany*

Integrated Motion Measurement Systems (IMMSs) are multi-sensor systems based on integrated navigation, which enable the traditional integrated navigation to be extended to capture deformations of an object as additional degrees of freedom (DOFs). Such systems comprise inertial sensors, i.e. accelerometers and gyroscopes, supported by aiding measurements from GNSS receivers or strain gauges, for example. To take advantage of these complementary sensors, an extended Kalman Filter (EKF) is used to acquire the conventional navigation states and the elastic DOFs. In case of elastic structures, it could be shown that these DOFs reflect the modal characteristics of the object, provided that the IMMS is modelled accordingly. Along with enhanced navigational performance, the additional system output can serve as an indicator for tasks such as Structural Health Monitoring (SHM).

Due to the technological advancement regarding micro-electro-mechanical systems (MEMSs) in recent decades, low-cost inertial sensors are now available in large quantities. Consequently, the application of small-scale and high-quality inertial sensors (particularly gyroscopes), which was previously considered cost-ineffective, has become more affordable. In parallel, the use of distributed accelerometers, in competition with gyroscopes, has become established in fields like Experimental Modal Analysis (EMA).

To validate and test IMMSs, a test rig with a movable, flexible beam was created. The beam represents an idealization of an aircraft wing, mast, or rotor blade and is equipped with a customary hybrid sensor system, consisting of Inertial Measurement Units (IMUs), strain gauges, and distance sensors.

This contribution presents the application and results of IMMSs on a suspended, clamped beam with base excitation. Advantages of distributed gyroscopes over accelerometers are first discussed on an Experimental Modal Analysis (EMA) for the present excitation type and frequency range of the relevant modes. Furthermore, it is shown that IMMSs can observe selected modal coordinates of the object in the time domain and that gyroscopes show a superior performance for the present setup.

**Investigation of the quasi-static shear behaviour of glass fibre reinforced plastics including fibre rotations and a nonlinear stiffness development**

Häusler, Stephan; Fink, Richard; Radtke, Lars; Sander, Manuela 09:10
*University of Rostock, Germany*

An accurate determination of shear properties is essential for the structural assessment of fibre-reinforced composites. Commonly applied standardised testing methods, such as DIN EN ISO 14129, rely on simplifying assumptions, including linear-elastic material behaviour or pure shear loading. Consequently, the validity of the derived material parameters is limited. To address these limitations in quasi-static material characterisations, an advanced evaluation methodology is presented, enabling a decoupled consideration of geometric and material nonlinearities.

The approach employs an iterative algorithm based on the Classical Laminate Theory (CLT) combined with experimental data acquired via Digital Image Correlation (DIC). Under load, the global deformation of the specimens induces rotations of the fibres. To account for this geometric nonlinearity, the calculated rotation angles are used to iteratively update the stiffness matrix in the CLT. In addition, an optimisation routine is applied to capture the material nonlinearity. The shear modulus and transverse stiffness are adjusted to minimise the deviation of the calculated strains from the measured strains, yielding the characteristic stiffness evolution during the load application.

To determine the shear strength, Puck's failure criterion is employed to account for the combined shear and normal stresses in this test setup. The onset of inter-fibre fracture is estimated by a slope-based criterion of the shear vs. transverse stresses, referring to literature values. Comparing these results with the results of the standardised method shows a correction in shear strength of approximately 10%, providing a more accurate representation of the material's load-bearing capacity.

**Mechanical Characterization of material-extrusion manufactured Mycelium-bound Composites with Biopolymer Lattice Reinforcement**

Panjalipoursangari, Narges (1); Müller, Wolfgang H. (1); Völlmecke, Christina (2)

*1: Continuum Mechanics and Materials Theory Group, Technical University of Berlin, Einsteinufer 5, 10587, Berlin, Germany*

*2: Stability and Failure of Functionally Optimized Structures Group, Technical University of Berlin, Einsteinufer 5, 10587, Berlin, Germany*

09:30

Mycelium, the filamentous root network of fungi, forms dense, interconnected structures capable of binding and reinforcing organic or synthetic substrates. Owing to its biodegradability, low environmental footprint, and ability to infiltrate porous materials, it is considered a promising component for sustainable and circular material systems [1, 2]. When integrated into 3D-printed biopolymer lattice frameworks, it can function as a bio-based infill influencing the local strut deformation response and subsequently the structural integrity as well as the overall mechanical response of such mycelium-bound composites [3].

This study examines how fungal mycelium interacts with three-dimensional periodic lattice structures abricated by Material-Extrusion Additive Manufacturing (MEX AM). Building on recent findings that ycelium can infiltrate porous PLA structures and alter their mechanical behavior [3], PLA lattices with systematically varied periodic architectures were inoculated, dried, and subjected to quasi-static compression using a ZwickRoell Z050 testing system. Full-field strain measurements were recorded via DIC to resolve deformation modes and localization phenomena. Complementary, microscopy was used to assess the spatial pattern of mycelial growth within the lattice topologies, enabling correlation between biological infill, geometric accessibility, and mechanical response.

The research addresses three principal questions. First, it investigates how mycelial grown infill influences the compressive mechanical performance of 3D-printed lattice structures. Second, it investigates how 3D-printing parameters and lattice design choices, such as pore size, infill strategy, and structural density, interact with mycelial growth and how these factors can be optimized to enhance the mechanical performance of the mycelium-bound hybrid structures. Third, it examines how lattice geometry influences the degree and spatial distribution of mycelial propagation within the printed architectures.

This work builds on previous findings regarding the influence of mycelium on additively manufactured polymer structures [3] and expands the understanding of bio-based hybrid materials. Recent studies, such as Sharma and Le Ferrand [4], further highlight the potential of mycelium-based 3D-printed structures for robust and thermally insulating applications. The present investigation therefore systematically examines how lattice geometry and mycelial growth interact and shape the mechanical performance of these sustainable hybrid materials.

[1] **Jones (2024):** Untersucht Myzelmaterialien aus Abfallstoffen und zeigt deren Potenzial für nachhaltige nicht- und semistrukturelle Anwendungen.

[2] **Appels et al. (2019):** Analysieren, wie Herstellungsparameter die mechanischen und feuchtigkeitsbezogenen Eigenschaften von Myzelkompositen beeinflussen.

[3] **Panjalipoursangari et al. (2025):** Zeigen, wie das Wachstum von *Fomes fomentarius* die mechanischen Eigenschaften von 3D-gedruckten PLA- und PLA/Hanf-Biopolymeren verändert.

[4] **Sharma & Le Ferrand (2025):** Entwickeln 3D-gedruckte Gyroidstrukturen, die starke und wärmeisolierende Myzelverbundwerkstoffe für nachhaltige Infrastruktur ermöglichen.

**Impact of mechanical preload on the behavior of piezoelectric multilayer actuators**

Riedel, Simon (1); Kapelke, Simon (1); Fidlin, Alexander (2)

*1: Physik Instrumente (PI) SE & Co. KG, Germany*

*2: Karlsruhe Institute of Technology (KIT)*

09:50

Piezoelectric multilayer actuators are widely used in positioning systems due to their high accuracy, high forces, and great reliability. Despite their resistance to compressive loads, these actuators are particularly susceptible to damage from tensile forces. High tensile forces can induce cracks in the ceramic insulation of the actuators, resulting in a significant reduction in their operational lifespan.

This vulnerability is especially pronounced in dynamically operated systems, where compensating for tensile forces through the application of mechanical preload becomes necessary.

Applying mechanical preload to the end faces of the actuator alters the boundary conditions, leading to shifts in the resonance frequencies. These changes are even more pronounced in actuators with cracks. The measured dynamic behavior of the actuators, both for intact and cracked ones, can be accurately replicated with linear simulations by introducing contact stiffness at the end faces and the crack faces of the actuator. This demonstrates that adjusting only the boundary conditions in the simulation is sufficient to represent the impact of mechanical preload on the real actuators.

Given that the lifespan of cracked actuators is notably reduced, understanding how mechanical preload affects their remaining lifetime is a critical area of ongoing research. This investigation is conducted experimentally, focusing on determining whether compressing a crack with mechanical preload can reduce its negative impact on the actuator's residual operational lifespan.

**Application of embedding and the Moore–Penrose inverse in nonlinear solid mechanics**

Flajs, Rado 10:10
*Faculty of Civil and Geodetic Engineering, University of Ljubljana, Slovenia*

This paper presents a new approach to describing body deformation in nonlinear solid mechanics. We consider the genuine formulation of the inclusive deformation mapping $\Phi$, which maps a domain from the space $R^n$ to a codomain in the space $R^m$, where the dimensions m and n necessarily differ, usually with $n < m$. Because m and n have different dimensions, the deformation gradient is not invertible, and its determinant is not defined. This generalization affects the kinematic, equilibrium, and constitutive equations. These challenges can be addressed using the Moore-Penrose generalized inverse. The expression for specific volume change must be revised. Nanson's equation for surface change takes a different form. The velocity gradient tensor and the rate of deformation tensor in the material description are altered. The material time derivative of the stretch tensor, obtained from the polar decomposition of the deformation gradient, should be calculated using the generalized inverse. The first and second Piola–Kirchhoff stress tensors should be expressed in terms of the Cauchy stress tensor in a new way. In the constitutive equations, a pseudoinverse deformation gradient appears in the spatial description. The pseudoinverse should also be used in appropriate FEM discretization. Theoretical derivations and selected practical examples in the paper demonstrate the essential role of the Moore-Penrose inverse.

## S05: Nonlinear Oscillations

Organizer(s): Capobianco, Giuseppe *(FAU Erlangen-Nürnberg)*
Breuling, Jonas *(University of Stuttgart)*

## S05.01: Nonlinear Oscillations

Date: March 17, 2026 08:30–10:30
Room: KII, M17.22
Chair(s): Capobianco, Giuseppe
Breuling, Jonas

### Quasiperiodic Motions – Theory, Methods, and Applications to Multi-harmonic Vibrations

Hetzler, Hartmut 08:30
*Universitat Kassel, Germany*

In standard approaches, vibrational analyses are usually based on assuming periodic motions, which allows for the application of a large number of established methods, such as shooting algorithms or harmonic balance approaches. Beyond classical textbook applications, these approaches have evolved into powerful numerical tools that enable the analysis of large-scale problems.
However, a wide variety of phenomena encountered in practical applications go far beyond this framework.

Processes originating from the superposition – and often interaction – of multiple such motions may produce multi-harmonic vibrations, which are usually quasiperiodic and may exhibit additional bifurcation phenomena such as synchronization or quenching. The underlying theory and the associated phenomena lie at the core of classical dynamics, have stimulated many areas of mathematics (e.g., ergodic theory, measure theory), and have led to sophisticated results such as Arnold tongues or the KAM theorem.

Despite their significant practical relevance, the available toolbox for the analysis of quasiperiodic motions remains rather limited and thus is still an active field of research.

In this contribution, the basic theory of quasiperiodic motions is summarized with focus on practical numerical analysis. A unified framework based on invariant manifolds is presented, encompassing different numerical approaches (multiharmonic shooting, multiharmonic balance, finite differences, etc.) and thus providing a suitable environment for a versatile numerical toolbox. It is emphasized that this framework naturally includes standard periodic motions as a special case.

Furthermore, current research topics are discussed, such as the detection of different routes to synchronizing bifurcations, and advanced numerical techniques involving adaptive meshing based on appropriate error estimators. These methods are illustrated through applications in rotor dynamics, power electronics, and astrodynamics.

### Continuation of periodic solutions in conservative systems leveraging the first integral of motion

Vogelei, Julian; Hetzler, Hartmut 09:10
*University of Kassel, Germany*

In engineering and science, one is often interested not only in a specific solution, but also in how that solution changes with respect to a system parameter (e.g. the excitation frequency). To numerically compute solutions for a varying system parameter, continuation methods are used.

In most cases, dissipative systems are analysed. Here, the continuation of periodic solutions requires the existence of an explicit parameter that can be varied during the continuation process. On the other hand, a dynamic system can be conservative, which is characterized by the existence of a first integral of motion. In contrast to dissipative systems, a family of periodic solutions typically exists even without the variation of an explicit parameter [1]. Consequently, established continuation algorithms cannot be applied directly to compute such families of periodic solutions.

To deal with that, existing techniques in the literature either introduce an artificial parameter or use a pseudoinverse (Moore-Penrose inverse) to solve the overdetermined system [1,2]. However, one of the disadvantages of both of these methods is that the continuation parameter (which does not even exist for the latter approach) cannot be used to control the start and end of a continuation. This contribution presents a strategy to extend the established continuation framework to conservative systems by incorporating the value of the first integral as continuation parameter.

**Bibliography**

[1] Jorge Galán-Vioque and André Vanderbauwhede. Continuation of Periodic Orbits in Symmetric Hamiltonian Systems. In: Bernd Krauskopf, Hinke M. Osinga, and Jorge Galán-Vioque, editors, *Numerical Continuation Methods for Dynamical Systems*. Springer, 2007.

[2] M. Peeters, R. Viguié, G. Sérandour, G. Kerschen, and J. C. Golinval. Nonlinear normal modes, Part II: Toward a practical computation using numerical continuation techniques. *Mechanical Systems and Signal Processing*, **23**(1):195–216, 2009. https://doi.org/10.1016/j.ymssp.2008.04.003

**Koopman-Hill: A frequency-based stability method for periodic solutions with closed-form error bound**

Bayer, Fabia; Leine, Remco 09:30
*University of Stuttgart, Germany*

The Koopman-Hill method offers an efficient approach for computational stability analysis of linear time-periodic systems in the frequency domain, and thereby also for the Floquet stability analysis of periodic solutions of nonlinear systems obtained using the harmonic balance method. In the Koopman-Hill method, the truncated Hill matrix, whose eigenvalues approximate Floquet exponents, is reinterpreted as an approximate matrix representation of the Koopman operator acting on the original linear time-periodic system. The original system's fundamental solution matrix can then be approximated using only one matrix exponential. The accuracy of the approach has previously been supported only by numerical evidence, lacking rigorous theoretical guarantees.
This work presents an explicit, closed-form error bound for the truncation error of the Koopman-Hill method, establishing a solid theoretical foundation for its application. The bound applies to linear time-periodic systems whose Fourier coefficients decay exponentially with a sufficient rate and is derived using constructive series expansions. The bound quantifies the difference between the true and approximated fundamental solution matrices and enables conservative but reliable inference of Floquet multipliers and stability properties.
Numerical examples illustrate the practical relevance of the bound and underscore its importance as the first rigorous theoretical justification for the Koopman-Hill method.

**An integrated approach for the computation of Floquet multipliers using the finite difference method**

Seifert, Alexander; Hetzler, Hartmut 09:50
*Engineering Dynamics Group, Department of Mechanical Engineering, University of Kassel, Germany*

The investigation of stationary periodic solutions is a standard task when determining the dynamic behavior of a system. The process can be subdivided into two main tasks. First, the calculation of the stationary periodic solution, generally using numerical methods. The second part is to determine the stability of the computed solution. This is done either by calculating the monodromy matrix and then determining the Floquet multipliers, or by directly computing the Floquet multipliers or exponents.

The standard procedure consists of integrating the linearized perturbation equation, with the periodic solution as reference, over one period T for orthogonal initial conditions. However, this requires additional computational effort after the periodic solution has been calculated. Furthermore, the Jacobian is often unknown and must be calculated separately. Depending on the numerical method, with which the periodic solution has been calculated, information from the calculation can be reused to determine the stability of the periodic solution. This is a standard approach, when using the shooting method. Here the monodromy matrix can be extracted as a by-product from the Jacobian matrix

of the Newton algorithm. When using the harmonic balance method, the Floquet exponents can be extracted from the Jacobian of the harmonic balance algorithm by using Hill's method.

The finite difference method is a very robust approach for calculating periodic solutions. The downside however is that there is no algorithm, which can reuse information from the solution process to determine the stability of the periodic solution. In this contribution we present an integrated algorithm which uses information from the finite difference method to determine the stability of the solution. Based on the method of Hsu, the computation of the monodromy matrix is reduced to a pure matrix multiplication, utilizing Runge-Kutta methods, requiring no additional computational effort. We demonstrate the algorithm on an academic example.

**Escaping Boundaries from Period-One Rotations in a Parametric Pendulum Harvester: The Role of Electrical Loading**

Novelli, Nico; Fidlin, Alexander
*Karlsruhe Institute of Technology (Department of Engineering Mechanics), Germany*

10:10

Parametric pendulum harvesters convert prescribed vertical base motion into pendulum dynamics and can, under suitable excitation, exhibit stable period-one rotations that are highly effective for energy extraction. A central difficulty is that the electrical load is not merely a readout of performance: through the generator torque it acts as an adjustable, velocity-proportional sink. Higher loading increases instantaneous electrical power, but it can also suppress the motion, shrink the capture basin of the rotating attractor, and ultimately trigger loss of rotation.

A rigid pendulum with viscous joint losses and a power take-off that produces a tunable damping torque during harvesting is considered. Starting from the full large-angle equations of motion with harmonic vertical heave, a non-dimensional electromechanical model is derived and existence and stability of period-one rotations are analyzed. Basin maps and integrity measures for rotations under both harmonic excitation and synthesized irregular "sea-like" inputs are computed, and the erosion of basin boundaries as electrical loading increases is quantified.

Constant and modulated electrical loading strategies are compared and existence–stability–integrity maps that quantify the power–robustness trade-off are derived. The results yield practical guidelines for sustaining period-one rotations while maximizing average harvested power.

## S05.02: Nonlinear Oscillations

Date: March 17, 2026 16:30–18:30
Room: KII, M17.22
Chair(s): Breuling, Jonas
Capobianco, Giuseppe

**Nonlinear Modeling from Experimental Data via Spectral Submanifold Reduction**

Haller, George
*ETH Zürich, Switzerland*

16:30

I discuss a dynamical systems alternative to neural networks in the data-driven modeling of nonlinear phenomena. Specifically, the recent concept of spectral submanifolds (SSMs) provides very low-dimensional attractors in virtually all dynamics problems. A data-driven identification of the reduced dynamics on these SSMs gives a mathematically justified way to construct accurate and predictive reduced-order models for solids, fluids and controls without the use of governing equations. I illustrate this on physical problems that include structural vibrations, fluid-structure interactions, hydrogel oscillations, plant dynamics and the model-predictive control of soft robots.

**Data-Driven Reduced-Order Modeling of Systems with Memory via Spectral Submanifolds**

Bettini, Leonardo (1); Yang, Haocheng (2); Yerrapragada, Karthik (2); Eriten, Melih (2); Haller, George (1) 17:10

*1: ETH Zurich, Switzerland*
*2: University of Wisconsin-Madison, USA*

In many areas of applied science, there is growing interest in increasingly complex systems. In this context, reduced-order models play a vital role in studying system behavior by lowering computational costs and enabling rapid parametric studies while preserving physical interpretability. This is particularly valuable when only data are available. Among the various model reduction techniques, we adopt the reduction on primary spectral submanifolds (SSMs), whose internal dynamics serve as reduced-order models of the system. SSMs constructed over the eigenspaces associated with the system's lowest modes attract all nearby trajectories and enable substantial dimensionality reduction.

However, modeling the dynamics of systems with memory effects, such as viscoelasticity and hysteresis, remains challenging, especially when no explicit constitutive laws are available. This situation commonly arises in soft materials, which combine solid-like and liquid-like properties. Such materials are increasingly used in biomedical applications due to their compatibility with biological tissues and in soft robotics for their compliance and adaptability to complex geometries. Their mechanical response depends not only on the current deformation but also on the history of loading, leading to phenomena such as creep, relaxation, and hysteresis.

In this work, we extend SSM-based model reduction to systems exhibiting memory effects, both in equation-based and data-driven settings. We show that memory effects leave clear signatures in the system's backbone and forced response curves. Although memory renders the system inherently infinite-dimensional, we derive a reduced-order model by augmenting the standard SSM-based formulation with an internal state that captures the material's memory dynamics and can be inferred directly from data. We validate the proposed approach using experimental data from vibrating hydrogels, demonstrating accurate prediction of both backbone and forced response curves with a nonlinear three-dimensional reduced-order model.

**Exact Principal Koopman Eigenfunctions of a Pendulum**

Römer, Ulrich J. 17:30

*TU Bergakademie Freiberg, Germany*

The Koopman operator provides a rigorous framework for representing nonlinear dynamics through linear (or bilinear) evolution in an appropriately chosen space of observables. For deterministic, dissipative systems the theory guarantees the existence of a global coordinate transformation that renders an autonomous system linear, and an input-affine system bilinear. Despite this powerful existence result, explicit constructions of the required observables are known only for a handful of elementary models, and most practical applications rely on data-driven approximations such as extended dynamic mode decomposition or kernel-based lifts. These methods typically increase the dimensionality of the state, introducing more coordinates than the original mechanical model.
In this contribution we revisit the classical damped, actuated pendulum as a benchmark for exact Koopman analysis. Building on the extension of the Hartman-Grobman theorem proposed by Lan and Mesić (2013), we identify a minimal set of principal Koopman eigenfunctions. For the autonomous pendulum we develop an algorithm that computes the exact transformation point-wise: given any state $(\Theta, d\Theta/dt)$ the algorithm yields the corresponding eigenfunction values and thus the linear coordinates. This procedure provides a globally valid mapping without the need for a higher-dimensional lift.
To incorporate actuation, we treat the input term as a perturbation of the autonomous dynamics. By applying a systematic perturbation expansion to the principal eigenfunctions, we obtain a point-wise evaluation of the bilinear representation of the forced pendulum. The algorithm delivers the bilinear coefficients for any prescribed state and input, preserving the original two-dimensional state dimension.
The algorithmic approach for the exact evaluation of the principal Koopman eigenfunctions can serve

as ground truth for the training of data-driven models. As an outlook, we plan to extend the method to higher-dimensional mechanical and robotic systems and to explore its use in systematic model-based controller design within the Koopman framework.

**Learning Duffing-Type Forces for the Harmonic Balance Method Using Neural Networks**

Goldack, Miriam (1); Groß, Johann (2); Krack, Malte (2); Stender, Merten (1)
*1: Cyber-Physical Systems in Mechanical Engineering, Technische Universität Berlin, Germany*
*2: Institute of Aircraft Propulsion Systems, University of Stuttgart, Germany*

17:50

Thin-walled lightweight structures often exhibit geometrically nonlinear behavior, which continues to pose challenges for accurate and efficient simulation. The Harmonic Balance Method (HBM) is a numerical simulation method and one of the most relevant approaches for modeling nonlinear structural dynamical systems. It represents the system response as a truncated Fourier series and effectively casts the equation of motion into the frequency domain. The main computational bottleneck is the evaluation of nonlinear forcing terms, for which the Alternating Frequency-Time (AFT) method is the standard approach. The AFT evaluates the nonlinear force in time domain and hence requires both an inverse Fourier Transform (FT) and a forward FT, which overall is computationally demanding.
In this work, we propose to replace the AFT with a neural network architecture trained for a specific type of contact nonlinearity, a cubic stiffness, and a fixed number of harmonics. It takes normalized Fourier coefficients of the displacement as input and outputs the corresponding nonlinear force Fourier coefficients without making use of the FT. Proof-of-concept studies on the Duffing oscillator demonstrate that the neural network can accurately learn the mapping and even provide the derivatives of the nonlinear forcing coefficients with respect to the displacement coefficients through automatic differentiation. The resulting Jacobian can then be used directly, leading to a more efficient and better-conditioned (iterative) solution process. Prediction errors are evaluated in terms of the data fit (i.e. matching coefficients computed by the AFT), but also in terms of the resulting system response (i.e. integrating the neural AFT into the classical HBM procedure).

## S05.03: Nonlinear Oscillations

Date: March 18, 2026 08:30–09:30
Room: KII, M17.22
Chair(s): Breuling, Jonas
Capobianco, Giuseppe

**Violoncello string vibrations as an example of continuum dynamics**

von Wagner, Utz; Gödecker, Holger
*Technische Universität Berlin, Germany*

08:30

*Vibrations in string instruments and especially the excitation of their strings by bowing or plucking have been subject of considerations and research since decades in textbooks (e.g. [1]) or research papers (e.g. [2]).*

*The current presentation collects some instructive measurement results with a violoncello and their interpretation in the framework of mechanical linear or nonlinear oscillations, respectively. We consider excitation mechanisms, boundary conditions, response spectra, flageolet harmonics, stick-slip limit cycles and compare strings idealized in the sense of Mechanics with real strings. We hope to give with the presentation some descriptive results for treatment within the context e.g. of lectures in continuum mechanics and friction excited vibrations.*

[1] Cremer, L.: The Physics of the Violin. MIT press 1984.

*[2] Akar, Ö.; Willner, K.: Investigation of the Helmholtz Motion of a Violin String: A Finite Element Approach. Journal of Vibrations and Accoustics, Vol. 142(5), DOI: 10.1115/1.4047417, 2020.*

**Transient Simulation of elastic foil structures in bump-foil bearings**

Schmidtchen, Fabian; Nitzschke, Steffen; Woschke, Elmar
*Otto-von-Guericke-University Magdeburg, Germany*

08:50

Bump-foil bearings represent a promising oil-free alternative to conventional oil-lubricated journal bearings in high-speed turbomachinery, particularly in the growing field of renewable energy systems. Their functionality is based on the elastic interaction between the top-foil and the bump-foil, which deform under the aerodynamic pressure field described by the Reynolds equation. This deformation, in turn, modifies the air gap and thus the resulting pressure field, creating a strongly coupled fluid-structure interaction. For transient simulations, typically more than $10^6$ evaluations of the describing force element are required, making an efficient numerical representation of the elastic structures essential.

In this work, the mass and stiffness matrices of the top-foil and bump-foil structures - generated in an FEM system using shell elements - are employed and supplemented by a contact algorithm to realistically capture the nonlinear interactions. The resulting system of equations has a large number of degrees of freedom; therefore, a suitable model reduction is performed to enable an efficient yet accurate representation of the structural deformations.

The developed algorithm is integrated into a transient overall simulation of the bump-foil bearing. This allows for a significantly more precise analysis of the time-dependent operating behavior of the bearing, contributing to improved design and assessment of oil-free bearing concepts.

**Self-Heating of Rubber Elements in Vibration Absorber Systems**

Niksirat, Esmat (1); Lindner, Markus (1); Kröger, Matthias (2)
*1: Jade Hochschule Wilhelmshaven, Germany*
*2: TU Bergakademie Freiberg, Germany*

09:10

The self-heating of rubber is a less understood topic, with only a few publications addressing it in the scientific literature. Vibration absorber systems are designed to reduce the movement of machines, vehicles, and other devices. When vibration absorbers include rubber elements, the vibration energy can be converted into heat due to the material dissipation properties.

This publication focuses on the self-heating of rubber by comparing measurements with numerical calculations of the internal heating within the rubber element. The material is simulated with respect to an internal, localized energy source. At the eigenfrequency of the basic system, the rubber mounting between the shaker test rig and the base heats up significantly, without the use of the absorber, due to the high vibration amplitude of the system.

Under the same performance conditions of the shaker test rig, but with the inclusion of the absorber containing rubber elements, the self-heating of the rubber mounting at the base is significantly reduced. This demonstrates the effectiveness of the absorber.

The main focus of this publication is the comparison of temperature measurements of the rubber components with numerical calculations. The simulation employs the finite difference method and shows a strong agreement with the experimental measurements.

In conclusion, this publication represents a unique contribution to the investigation of the self-heating of rubber elements, aiming to enhance scientific understanding of this phenomenon.

## S05.04: Nonlinear Oscillations

Date: March 18, 2026 14:00–16:00
Room: KII, M17.22
Chair(s): Capobianco, Giuseppe
Breuling, Jonas

**Mechanics of the golf lip out, including the golf balls of death**

Hogan, Stephen John
*University of Bristol, United Kingdom*

14:00

Many golfers have experience of the lip out ("the golfer's curse"): you are on the 18th hole, and the match is almost won. You line up your putt, take a breath, and roll the ball toward the hole. The pace is firm, the line looks good—until the ball dips in, then cruelly pops back out onto the green.

We consider the problem from the point of view of mechanics. We show analytically that there are at least two distinct types of lip out: the rim lip out, where the centre of mass of the golf ball does not fall below the level of the green, and the hole lip out where it does. At the heart of both lip outs is a family of degenerate saddle equilibria of the dynamics on the rim (the "golf balls of death" whose motion is reminiscent of a famous fairground attraction). When perturbed one way, the golf ball executes a rim lip out. When perturbed another way, the golf ball enters the hole, only to re-emerge if it is spinning about an axis perpendicular to the wall of the hole (provided it does not touch the base of the hole).

Reference: Hogan, S.J. and Antali, M. Mechanics of the golf lip out. R. Soc. Open Sci. 12, 250907 (2025) https://doi.org/10.1098/rsos.250907

This article has received an enormous amount of media coverage, from all around the world, including interviews on NPR in the USA and CBC in Canada. If time permits, I will speak a little bit about my dealings with the media.

Joint work with Máté Antali, Department of Applied Mechanics, Szechenyi Istvan Egyetem, Győr, Gyor-Moson-Sopron, Hungary

**Numerical bifurcation analysis of nonsmooth periodic solutions**

Wagemakers, Lara
*University of Antwerp, Belgium*

14:20

This talk introduces key ideas and tools needed to perform a numerical bifurcation analysis of nonsmooth dynamical systems. In a bifurcation analysis, we track how solutions and their stability change as physical parameters of the system are varied. Doing so provides insight into the overall solution landscape. The nonsmooth systems we consider are differential equations with coupled complementarity conditions involving inequality constraints. Unique challenges arise due to the nonsmoothness, such as the calculation of the monodromy matrix for determining the stability of periodic solutions. As demonstration, we will walk through the first steps in the numerical continuation and stability analysis of periodic solutions of a conceptual model for the Atlantic Meridional Overturning Circulation (AMOC), formulated as a Filippov system.

**Oscillations of a moving bandsaw blade in a narrow lubricated gap**

Scheidl, Jakob; Steindl, Alois; Strondl, Manuel
*TU Wien, Austria*

14:40

We investigate the linear stability of a moving bandsaw blade in a narrow lubricated kerf. Assuming that the fluid problem is governed by Reynold's lubrication theory, we study the influence of static and oscillating cutting forces, as well as periodically varying pre-tension forces on the stability of the steady axially moving blade and the bifurcating oscillations.

**Prediction of Crater Formation in Impact Energy Scatterers**

Madhikarmi, Krishaa; Waschinsky, Navina; Ricken, Tim 15:00
*Institute of Structural Mechanics and Dynamics in Aerospace Engineering (ISD), University of Stuttgart, Germany*

Impact energy scatterers (IES) are passive vibration-mitigation devices in which a small auxiliary mass is attached to a host structure. Their operating principle is theoretically based on the transfer of vibrational energy from low-frequency structural modes to higher frequencies through repeated impacts, while only minimal energy is dissipated at the contact interface. Each impact, however, is accompanied by localized deformation of the cavity walls of the host structure, and a crater is gradually formed. The evolution of this crater modifies the effective contact stiffness between the mass and the host structure and thereby alters the overall damping performance.
In this work, a simplified dynamic model for successive sphere–wall impacts is proposed, which captures the progression of crater formation in an inelastic wall. Material parameters governing plasticity are subsequently optimized so that experimentally observed crater depth and shape are reproduced. In addition, an uncertainty-quantification analysis is carried out to assess the influence of variability in the material parameters on the predicted crater depth and shape. The resulting prediction methodology is shown to be in strong agreement with experimental results and numerically derived effective contact stiffness, thereby validating its capability to reliably forecast crater formation in inelastic walls.

**Influence of permeability and thickness of the porous layer in the porous air bearing on stability and load-bearing capacity**

Stellmach, Laurenz; Nitzschke, Steffen; Woschke, Elmar 15:20
*Otto-von-Guericke University Magdeburg, Germany*

Due to the growing demands in the semiconductor industry and the associated requirements for manufacturing machines, the simulation of these machines and their components is essential in order to enable smaller structure widths in production. The bearing of the moving components is essential, which, due to the requirement for purity, is achieved by means of air bearings. Components that operate in the low speed range are usually supported by porous air bearings, which operate with low friction and high precision thanks to an external air supply.
The paper deals with the simulation of this kind of bearings by solving the Reynolds and Darcy equations in conjunction with the continuity equation. To find the solution, the solution area is discretized using the finite volume method. Since the partial differential equations are nonlinear, the Newton-Raphson method is implemented to find the solution quickly and reduce the time required for individual force element calls during time integration.
In this porous air bearings it can be seen that the permeability and thickness of the porous bearing shell have a very large influence on stability. The extent of the influence of these two parameters and how they interact with each other is studied.
From a manufacturing point it is easier to adjust the thickness than the permeability. Hence, more attention is paid to this variable in this study.

**An Efficient Rotordynamic Model for Investigating Slow and Heavy Flywheel Energy Storage Systems**

Juwailes, Yousef; Beitelschmidt, Michael 15:40
*Technische Universität Dresden, Germany*

Due to the increasing use of volatile renewable sources for generating electrical energy, storage systems on various time scales are becoming increasingly important. To that end, mechanical energy storage systems that utilize rotating flywheels as their storage medium have gained research and commercial interest in recent years. One configuration is the slow-speed and heavy steel flywheel system, typically operating at 3000 rpm. This speed-mass combination necessitates careful rotordynamics analysis to ensure safe operation. Such analyses typically involve meshed models with many degrees of freedom, leading to large system matrices that must be inverted to calculate the system response to excitation. In this work, an analysis approach is put forward, that employs a very small

number of classical massless elastic beam elements in combination with rigid disk(s). The model's performance is benchmarked against two reference models: a typical model with 3D volume elements created using Ansys, and a beam-element-based model found in the literature. Modal and time-domain simulations are carried out to assess performance. Despite the reduced complexity, the proposed model achieves results comparable to the first benchmark, and almost identical results to the second.

## S06.1: Material modelling with metals

Organizer(s): Kaiser, Tobias *(TU Dortmund University)*
Klusemann, Benjamin *(Leuphana University Lüneburg)*

### S06.1.01: Temperature-induced and thermally affected processes

Date: March 18, 2026 14:00–16:00
Room: KI, M11.82
Chair(s): Klusemann, Benjamin
Kaiser, Tobias

**Computational Chemo-Mechanics with Application to High-Temperature Materials**

Kiefer, Björn; Prüger, Stefan; Roth, Stephan 14:00
*TU Bergakademie Freiberg, Germany*

This contribution gives an overview of our current research activities in the area of chemo-mechanics-based material modeling. Building on experience in theoretical and computational methods for multiphysics problems, our interest here lies in the modeling of nonlinear, dissipative material behavior in which interacting thermo-chemo-mechanical processes play a dominant role. We aim to capture mechanisms such as stress- and temperature-biased phase transitions and chemical reaction-diffusion processes that directly influence, or even enable, the effective behaviors of modern engineering materials. In this general multiscale approach, model formulations may be considered on very different length and time scales. Recent work regarding analytical and computational scale-bridging methods is also briefly discussed.

Three fundamental ingredients are addressed in this talk: (i) the theoretical model development, particularly regarding variational settings, (ii) the numerical treatment of these problems and the corresponding high-performance computing approach, and (iii) the calibration of thermodynamical properties via the CALPHAD method. Regarding the first aspect, we discuss the advantages and disadvantages of formulations for chemo-mechanical multifield problems through minimization and saddle-point principles. In terms of numerical solution schemes, we elaborate on the finite element implementation of such theoretical frameworks. Our particular approach builds on the flexible and quite general utilization of the UserELement interface (UEL) provided in the FE software package Abaqus. We further discuss ongoing collaborative work on the co-design of the variational model development and parallel solvers for chemo-mechanics problems, for which the MPI-parallel implementation instead is based on the software libraries deal.II, p4est and FROSch (Fast and Robust Overlapping Schwarz). Moreover, a concept is proposed in which thermodynamically informed material models are efficiently achieved via CALPHAD-trained neural networks. Representative numerical examples from a broad spectrum of technologically relevant studies — ranging from high-temperature electrolyzers to multifunctional filters for the cleaning of steel melts — are presented to demonstrate the validity and flexibility of our simulation frameworks.

References:

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[2] Seupel, A., Roth, S. and Kiefer, B., 2023. Phase-Field Modeling of Chemically Reactive Multi-Component and Multi-Phase Systems, Proc. Appl. Math. Mech. 22(1), e202200154.

[3] Kiefer, B., Prüger, S., Rheinbach, O. and Röver, F., 2022. Monolithic Parallel Overlapping Schwarz Methods in Fully-Coupled Nonlinear Chemo-Mechanics Problems, Comput. Mech. 71, 765-788.

**A thermodynamically consistent large-strain framework for microstructure-informed thermomechanical processing**

Böddecker, Merlin (1); Menzel, Andreas (1,2) 14:40

*1: Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Dortmund, Germany*
*2: Division of Solid Mechanics, Department of Construction Sciences, Lund University, Lund, Sweden*

Microstructural tailoring through thermomechanical processing steps such as hot working and annealing plays a key role in achieving favourable combinations of macroscopic material properties, including strength, ductility, and formability. The associated temperature-activated metallurgical mechanisms - work hardening, recovery, recrystallisation, and grain size evolution - are governed by the stored energy of plastic deformation, i.e. dislocation density, and grain boundary energy. Their interaction results in softening, as dislocation rearrangement and the formation of recrystallised, dislocation-free regions reduce the hardening state, while grain size evolution modifies the strength through the Hall-Petch effect. For reliable process design and simulation-supported optimisation, constitutive descriptions are required that represent these coupled mechanisms in a unified manner and, beyond stress-strain prediction, provide microstructural state information relevant for subsequent forming steps.

In Cho et al. [1], a recrystallisation-based hardening formulation is proposed within a hypo-elastic large-strain thermoplasticity framework, unifying the interdependent effects of recovery, recrystallisation, and grain size evolution under static and dynamic loading conditions. To overcome the limitations of hypo-elastic formulations at large strains, the recrystallisation-dependent hardening description is embedded into a fully thermomechanically coupled, thermodynamically consistent hyperelastic-plastic framework [2]. The formulation is based on a multiplicative decomposition of the deformation gradient and an isotropic, temperature-dependent hyperelastic law defined in logarithmic strains. Plastic flow is governed by a temperature-dependent von Mises yield condition, while the hardening response is formulated in a hardening-minus-recovery structure derived from recrystallisation-dependent plastic potentials, with the hardening variable interpreted as a dislocation-density-related quantity. Microstructural state variables describing the recrystallised volume fraction and the average grain size are incorporated within the hardening description, and their evolution is driven by physically meaningful driving forces associated with temperature, stored deformation energy, and grain boundary energy via Arrhenius-type activation functions. The thermodynamically consistent structure yields intrinsic constraints on the coupled internal variable evolution and establishes a robust basis for predicting softening and microstructural state changes under sequential thermomechanical loading. The microstructure-informed framework is essential for describing healing effects during recrystallisation and for downstream modelling, where initial microstructural conditions govern the subsequent mechanical response, including damage evolution.

**References**

[1] H. Cho, Y. Hammi, A. Bowman, S. Karato, J. Baumgardner and M. Horstemeyer, "A unified static and dynamic recrystallization Internal State Variable (ISV) constitutive model coupled with grain size evolution for metals and mineral aggregates", *Int. J. Plast.*, 112:123-157, 2019.
[2] M. Böddecker and A. Menzel, "A large strain thermoplasticity model including recovery, recrystallisation and grain size effects", *Proc. Appl. Math. Mech.*, 23(4):e202300282, 2023.

**Simulation of High-Pressure-Torsion within the Material-Point-Method using Periodic Boundary Conditions**

Cloidt, Dominik-Oliver; Schröder, Jörg 15:00

*University of Duisburg-Essen, Germany*

This study focuses on simulating the high-pressure torsion process, with particular emphasis on the heterogeneous microstructure under extreme plastic deformations. The Material-Point-Method, a mixed Eulerian-Lagrangian approach, proves highly suitable for boundary value problems involving

large deformations and dynamic processes, as it avoids mesh entanglement issues associated with standard Lagrangian methods.

High-pressure torsion is a thermomechanical forming process where material samples undergo extreme hydrostatic pressure combined with progressive torsional deformation. This combination generates a nanocrystalline microstructure featuring enhanced mechanical properties—such as greater strength and ductility—through severe shear straining. Given the substantial deformations involved, the Material Point Method offers an ideal framework for analyzing and understanding this process.

Periodic boundary conditions are employed to account for the underlying micromechanical phenomena. The microstructure is examined under various stress states through convergence studies. Oscillations can be effectively mitigated using either the B-Bar method or grid-shift techniques. Throughout these investigations, microstructural phenomena—such as grain refinement—are evaluated, providing valuable insights into the failure mechanisms of microstructured metals.

**Arbitrary Lagrangian-Eulerian formulation in a rotating frame to model friction spinning**

Friedlein, Johannes; Steinmann, Paul; Mergheim, Julia 15:20
*Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of Applied Mechanics, Germany*

The arbitrary Lagrangian-Eulerian (ALE) method allows to decouple the material motion from the deformation of the finite element mesh. This enables to simulate processes with large deformations and rotations.

Friction spinning is such a process, where a metallic workpiece rotates rapidly relative to a blunt tool whilst being formed freely. The high velocity in the contact interface leads to friction-induced heating. This heat conducts into the workpiece causing thermal softening, which enables an easier and more permissive deformation of the workpiece. Thereby various shapes can be manufactured. Friction spinning can also be used to produce rivets, so-called friction-spun joint connectors (FSJC), and to join components.

A computational model is presented using the finite element method to simulate the forming and joining by FSJC. Thereby, several challenges arise due to the special process characteristics.

The frictional heating induces thermal softening, which allows for extreme deformations. Moreover, the high temperature gradients at the contact interface cause strongly localised deformations. This is here captured by the ALE formulation, which allows for controlled smoothing of the underlying Lagrangian mesh.

The rapid spinning at around 10000 rpm also need to be captured efficiently. This is realised by decoupling the rotational motion from the (axisymmetric) mesh deformation/motion fitting well into the above ALE framework.

The frictional heating brings the process temperature close to the workpiece's melting point. Consequently, the material undergoes a wide temperature range (e.g. 20 °C to 1500 °C for steel), which demands suitable constitutive models. These are equipped with material properties calculated by JMatPro (CALPHAD-method) to span this large process window.

**Full-field identification of the Taylor-Quinney factor in copper tensile tests via in-situ infrared thermography**

Lalovic, Nikola; Böhlke, Thomas 15:40
*Institute of Engineering Mechanics - Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT), Germany*

Accurate thermo-elasto-plastic modeling requires simultaneous capture of mechanical and thermal responses. However, conventional identification strategies often depend on localized point measurements, which fail to resolve spatially varying phenomena. To meet growing interestin spatially resolved analysis, this study employs in-situ infrared thermography (IRT) to identify dissipative and energetic components during monotonic, quasi-static tensile testing of oxygen-free copper.

Grounded in a thermodynamically consistent framework, the flow stress is decomposed into energetic and dissipative components, enabling derivation of the Taylor-Quinney factor, i.e., the inelastic heat conversion rate [1]. IRT-derived thermal fields are processed to reconstruct the spatially distributed heat source [2], which is then coupled with phenomenological plasticity model fitting [3].

This dislocation-based theoretical approach offers insights into how energy and stress partition during plastic deformation. By enabling full-field identification of the Taylor-Quinney factor, the study advances fundamental understanding of the heterogeneous, discrete, and dissipative nature of plastic flow in metallic materials, and establishes a foundation for future investigations into thermomechanical-microstructural couplings. Representative experimental results obtained by multiple identification strategies, are presented, along with current limitations and potential directions for methodological refinement.

[1] Gurtin, Morton E., Eliot Fried, and Lallit Anand. *The Mechanics and Thermodynamics of Continua*. 1st ed. Cambridge University Press, 2010.

[2] Chrysochoos, A., & Louche, H. (2000). An infrared image processing to analyse the calorific effects accompanying strain localisation. *International journal of Engineering Science*, *38*(16), 1759-1788.

[3] Lalovic, N., Dyck, A., Kauffmann, A., Heilmaier, M., Estrin, Y., Böhlke, T. (2025). Experimental analysis of a thermodynamically motivated decomposition of plastic flow stress. Manuscript submitted for publication.

## S06.1.02: Strain ageing, creep and additive manufacturing

Date: March 19, 2026 14:00–16:00
Room: KI, M11.82
Chair(s): Waimann, Johanna
Kaiser, Tobias

### Analysis and modelling of ageing time evolution during non-monotonous loading paths within Dynamic-Strain-Ageing models

Rose, Lars (1); Menzel, Andreas (1,2) 14:00
*1: Institute of Mechanics, TU Dortmund University, Germany*
*2: Division of Solid Mechanics, Lund University, Sweden*

Dynamic Strain Ageing (DSA) and the associated Portevin-Le Chatelier (PLC) effect continue to pose challenges for constitutive modelling, particularly when load paths deviate from simple monotonic deformation. Many established modelling approaches, including those based on the Estrin-McCormick framework, rely on an ageing-time variable that represents the diffusion based interaction between solutes and dislocations. While this concept allows the reproduction of characteristic DSA features, the classical evolution equation proposed by McCormick does not specify under which mechanical conditions the ageing time should accumulate. As a result, ageing-time evolution is typically assumed to proceed continuously, which may lead to non-physical hardening contributions in simulations involving holds, unload-reload sequences, or other non-monotonous loading scenarios.

The aim of the talk is to address this issue by combining experimental results and modelling considerations. To do so, tensile tests with defined waiting times are presented for the aluminium alloy AW5083. These experiments were designed to quantify strain ageing during distinct deformation stages and to assess the influence of applied stress during brief waiting intervals on the subsequent material response.

Based on these observations, a modified evolution equation for the ageing time is proposed. The formulation maintains the fundamental structure of the Estrin-McCormick approach but restricts ageing-time accumulation to states in which the mechanical conditions support ageing processes, as suggested by the experiments. This prevents the unintended growth of DSA-related strengthening that can occur in the classical formulation, without increasing the complexity of the constitutive model.

A comparison between simulations using the classical and the modified approach shows that both reproduce the general characteristics of the PLC effect. However, the enhanced model yields more consistent results for
non-monotonous loading paths and provides a closer alignment with the experimental findings for AW5083. The presented work therefore offers a practical refinement for the use of DSA models in finite element simulations
where realistic load histories must be represented.

**Automated Formulation of Advanced Creep–Fatigue Constitutive Models Using Query-Based Decision Systems**

Jahnke, Alexander (1); Riepin, Bohdan (1); Naumenko, Konstantin (1); Kostenko, Yevgen (2) 14:20

*1: Otto-von-Guericke Universität Magdeburg, Germany*
*2: Siemens energy, Germany*

Mechanism-based constitutive models for creep–fatigue analysis, together with the corresponding user material subroutines for finite element codes, have been developed by numerous research groups over recent decades. However, their industrial application remains limited due to the need for extensive high-quality experimental data, the time-intensive parameter identification process, and the specialized expertise required to construct such models.

This presentation introduces an automated workflow *Get Constitutive Model* for developing advanced mechanism-based constitutive models for 9–12% Cr heat-resistant steels. The workflow enables blockwise model construction and automated material parameter identification using artificial neural networks (ANNs). Model generation and ANN training are implemented in Python using the Keras and TensorFlow machine-learning libraries. To evaluate the resulting constitutive model, the Simcenter Nastran environment is employed with a dedicated NXUMAT user subroutine.

Model predictions are validated against experimental data across a range of applied stresses and temperatures. The robustness of the subroutine in handling variable mechanical and thermal loads, as well as complex geometries, is assessed through low-cycle fatigue (LCF) and thermomechanical fatigue (TMF) simulations. Additionally, the capabilities of the model are demonstrated through analyses of a steam-turbine rotor and an inner casing subjected to realistic operating conditions. Representative benchmark tests and component-level case studies are presented to illustrate the effectiveness of the proposed approach.

**Three-Scale Homogenization of Lamellar NiAl-(Cr,Mo) Composites**

Klein, Claudius (1); Vollhüter, Jan (2); Neumeier, Steffen (2); Kauffmann, Alexander (3); Böhlke, Thomas (1) 14:40

*1: Karlsruhe Institute of Technology (KIT), Germany*
*2: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*
*3: Ruhr University Bochum, Germany*

The macroscopic mechanical response of composite materials depends on the properties of the constituents as well as the microstructure, i.e., the spatial arrangement of the constituents. In this talk we focus on the high temperature creep response of a eutectic NiAl-(Cr,Mo) composite [1], which forms domains (eutectic colonies) within which two metallic phases are arranged as ultra-fine lamellar structures. Mesoscopic creep experiments of individual colonies showed that the minimum creep rate spans several orders of magnitude depending on the load direction relative to the lamination direction. The apparent Norton exponent also shows a strong anisotropy. Both effects are due to an inhomogeneous stress partitioning between the two phases which originates from the lamellar morphology and the high material contrast.

In order to model the macroscopic mechanical response of the material system, we make use of a three-scale homogenization scheme involving two length scale bridges. For this, we describe the lamellar microstructure as a periodic rank-1 laminate [2], which allows for an efficient evaluation of the effective behavior of a single colony. To account for the interaction between different colonies, we use numerical homogenization techniques, e.g., the description of the mesostructure as a Laguerre

tesselation [3] with prescribed lamination orientation and its discretization using finite elements. After identification of the constitutive laws of the single phases, we compare the effective simulated behavior to experimental data as an interim result.

References:

[1] Gombola, C. et al., Microstructural Investigations of Novel High Temperature Alloys Based on NiAl-(Cr,Mo). Metals 2020, 10, 961.

[2] G.W. Milton, The Theory of Composites (1995), Chapter 9, Cambridge University Press, Cambridge

[3] J. Kuhn et al., Fast methods for computing centroidal Laguerre tessellations for prescribed volume fractions with applications to microstructure generation of polycrystalline materials, Comput Methods Appl Mech Engrg 2020, 369, 113175.

**Modelling Laser Metal Deposition with the Particle Finite Element Method and a large strain temperature-dependent viscoelastic material model**

Olatunbosun, Justice (1); Schewe, Markus (1); Bartel, Thorsten (1); Menzel, Andreas (1,2)

*1: Institute of Mechanics, TU Dortmund, Germany*
*2: Division of Solid Mechanics, Lund University, Sweden*

15:00

Laser metal deposition belongs to the family of metallic 3D printing under the directed energy deposition processes, with a laser beam as its energy source, abbreviated as the DED-LB process. The process is heavily utilised in the manufacture of metallic parts, featuring applications such as the repair of components, surface enhancement against corrosion, the formation of new parts – particularly for rapid prototyping – and its use in hybrid manufacturing.

Owing to the intricacies involved in the process, such as the specification of optimal printing parameters to achieve a desired weld-track geometry and the susceptibility of such tracks to residual stresses, frameworks that can predict these outcomes beforehand are being put forward to avoid material wastage. In this context, one approach is the Particle Finite Element Method (PFEM). The PFEM can readily capture the domain of rapidly evolving fluid surfaces due to its dynamic remeshing procedure. In addition, the offered remeshing technique enables a simplified, perfect-stick bonding between the interfaces of the hot flowing deposited melt and the substrate body without requiring a standard contact formulation. Such a modelling framework is presented for 2D in [1] and the mesh treatment methods are extended to 3D in the present contribution.

The flow and solidification behaviour of the hot metal involved in the process can be captured by using a temperature-dependent viscoelastic model. Based on the Maxwell fluid model, this viscoelastic formulation is able to reproduce the flow behaviour of the molten metal, while the associated material parameters can be coupled to temperature to represent solidification from the melt regime to the solid regime.

The goal of this work is to demonstrate, through a PFEM framework combined with a temperature-dependent viscoelastic model, the influence of specified printing parameters on the geometry of weld tracks formed by laser metal deposition and on the evolving heat distribution during the process. These findings will serve as a basis for improvement of the DED-LB process in a future work.

**References**

[1] M. Schewe, I. Noll, T. Bartel, and A. Menzel (2025) Towards the simulation of metal deposition with the Particle Finite Element Method and a phase trans-formation model. Computer Methods in Applied Mechanics and Engineering 437:117730. https://doi.org/10.1016/j.cma.2025.117730.

## S06.1.03: Numerics and coupled processes

Date: March 19, 2026 17:30–18:30
Room: KII, M17.14
Chair(s): Hellebrand, Sonja
Kaiser, Tobias

**Two-Stage Newton Algorithm for Magnetic Constitutive Models with Hysteresis**
Aliyeva, Ainura; Wulfinghoff, Stephan
*CAU Kiel, Germany* 17:30

We present a local constitutive solver for rate-independent vector magnetic hysteresis based on an incremental potential with a dissipation-controlled activation condition. The magnetization increment is computed by a two-stage Newton procedure: a scalar step enforces the activation condition and provides the initial magnitude, followed by a vector step that determines the full update. Numerical tests with linear and nonlinear Langevin-type magnetic laws show stable convergence under large changes of the applied field and accurate hysteresis loops.

**3D Simulation of Niobium-based Ferroelectric Materials with Precipitation Hardening**
Bohnen, Matthias; Müller, Ralf
*Technical University Darmstadt, Germany* 17:50

Our work is based on a phase field approach to simulate the evolution of domains in ferroelectric material. In particular we are focusing on materials with orthorhombic crystal symmetry, namely $NaNbO_3$, which exhibit 12 admissible polarization directions in three dimensions. We present a novel approach to define a phase field potential to model the microstructure with the desired symmetry. The model is formulated in three dimensions as the orthorhombic symmetry does not allow for plane formulations anymore.

Precipitation hardening has emerged as a new approach to enhance the mechanical properties of ferroelectric material, as recent studies have shown. As an alternative to doping, it effectively reduces domain wall mobility as well as heat dissipation. We are furthermore investigating the material system of NaNbO3 with LiNbO3 particles, where the orthorhombic ferroelectric is combined with precipitates of hexagonal symmetry. The interaction between matrix and precipitate produces new microstructure phenomena, contributing to the development of a new generation of ferroelectric material.

## S06.1.04: Crystal plasticity and dislocation densities

Date: March 20, 2026 08:30–10:30
Room: KII, M17.14
Chair(s): Wulfinghoff, Stephan
Kurzeja, Patrick

**An Augmented Lagrangian Formulation of General, Non-Associative Multi-Surface Plasticity at Finite Deformations**
Prüger, Stefan; Kiefer, Bjoern
*Technische Universität Bergakademie Freiberg, Germany* 08:30

The class of constitutive models that describe the inelastic behavior of engineering and natural materials by means of internal state variables and a set of limit surfaces is commonly employed as a standard tool in many engineering applications. However, the coupling of multiple irreversible phenomena, such as plasticity, damage and phase transformation, in these constitutive models typically requires the introduction of multiple independent coupled limit functions, cf. [1]. As the intersection of all limit functions defines the space of admissible stresses and thermodynamic driving forces, the boundary of the set of admissible states is not necessarily smooth. Consequently, singular points and edges emerge, at which the normal onto the limit surface is not uniquely defined, like in the classical Tresa and Mohr-Coulomb criteria. The complexity is further increased, if the evolution of the internal state variables is controlled by additional inelastic potentials, distinct from the limit functions, rendering the flow rule non-associative. These characteristics are well established in plasticity models of soils and rocks to accurately describe their distinct behavior in tension and compression and in crystal plasticity models.

Rather than applying a smoothing technique at the intersections of different limit surfaces [2] or exploiting the particular structure of simple limit surfaces [3], we propose a robust implementation of a general isotropic, non-associative multi-surface plasticity model at finite deformation based on the principle of maximum dissipation. Adopting the idea of introducing an additional state-dependency in the set of admissible stresses and thermodynamic driving forces [4], the principle of maximum dissipation holds, even in the non-associated case. Thus, the constrained optimization problem can be expressed by an Augmented Lagrangian formulation, in which arbitrary isotropic limit surfaces and inelastic potentials are allowed to intersect in a non-smooth manner, in particular giving rise to non-planar intersection curves. The implementation discussed in this contribution is an extension of our previous work on single crystal plasticity [5]. The robustness of the current implementation will be demonstrated both by means of material point and representative finite element simulations employing the Abaqus UMAT interface.

[1] B. Kiefer, et al., Int J Damage Mech, 27(2), 253–295, 2018.
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[3] J. Clausen, et al., Int J Numer Meth Eng, 66(6), 1036–1059, 2006.
[4] J. Ulloa, et al., Int J Solids Struct, 217–218, 272–296, 2021.
[5] S. Prüger and B. Kiefer, Int J Mech Sci, 180, 105740, 2020.

**Crystal plasticity modeling based on a single effective yield function**

Niehüser, Alexander; Mosler, Jörn
*TU Dortmund University*

08:50

Crystal plasticity theory provides a powerful framework for analyzing plastic deformation across different scales while explicitly incorporating crystallographic information into constitutive models. Classic crystal plasticity models are formulated using multi-surface yield criteria, in which the resolved shear stress on each individual slip system may not exceed a critical value. Unfortunately, these approaches face long-standing challenges regarding the determination of active slip systems and the computation of non-unique solutions due to linearly dependent constraints.

To overcome these challenges, a constraint aggregation approach may be utilized that reduces the multi-surface yield criterion into a single effective yield function. It is expected that this re-formulation will have a regularizing effect on the resulting system of equations and, thus, allows for a faster solution scheme. Two effective yield functions based on exponential-type functions – specifically the Log-SumExp function [1] and the p-Norm [2] – have already been used for hypo-elastic crystal plasticity models. However, these models systematically under-predict the stresses – which is non-conservative from an engineering point of view – and thermodynamic consistency is not necessarily ensured especially for moderate exponents. Therefore, these effective yield functions are adapted to a hyper-elastic framework and modified such that the predicted stresses are guaranteed to be larger than those in the classic model, and thus remain a conservative prediction from an engineering point of view. Furthermore, the asymptotic convergence to the classic crystal plasticity model is retained. Thermodynamic consistency of the resulting models is proven using the Generalized Standard Materials (GSM) framework. The resulting system of equations is well-conditioned, and thus may be solved by a standard Newton scheme. In order to further increase the efficiency of the solution scheme, different predictors for the Newton scheme will be discussed as well. Finally, numerical studies compare these effective formulations to a full multi-surface formulation solved by an augmented Lagrangian method [3], highlighting its improved efficiency.

References:
[1] A. Zamiri, F, Pourboghrat: A novel yield function for single crystals based on combined constraints optimization. International Journal of Plasticity, 26 (2010) 731-746.

[2] T. Mánik, H.M. Asadkandi, B. Holmedal: A robust algorithm for rate-independent crystal plasticity. Computer Methods in Applied Mechanics and Engineering, 393 (2022) 114831.

[3] A. Niehüser, J. Mosler: Efficient augmented Lagrangian algorithms for rate-independent crystal plasticity models. Computer Methods in Applied Mechanics and Engineering, 449 (2026) 118525.

**Accelerated interior point algorithms for rate-independent single-crystal plasticity at large strains**

Steinmetz, Felix; Scheunemann, Lisa 09:10
*RWTH Aachen University, Germany*

Crystal plasticity models describe the anisotropic behavior of metals by resolving plastic deformation on individual crystallographic slip systems. It is well known that the rate-independent formulation poses algorithmic challenges due to the non-uniqueness of active slip systems, demanding efficient numerical algorithms [1].

Recently, new formulations based on interior point methods have emerged. Among them, the primal-dual interior point method is a promising approach, where logarithmic barrier functions are incorporated into the objective function to enforce the inequality constraints [2,3]. This regularizes the problem, and gradually reducing the barrier parameter while applying Newton iterations allows recovery of the solution to the original problem.

A major drawback of interior point methods is their nested loop structure: the outer loop reduces the barrier parameter while the inner loop solves the barrier subproblem. This significantly increases computational cost and hinders the efficient warm-starting within FEM simulations. We address this limitation by adopting a fixed barrier parameter and exploiting information from previous load steps to initialize subsequent solves, enabling efficient warm-starting. We demonstrate the efficiency and robustness of the proposed approach through numerical examples at both the material point level and in FEM simulations.

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**Scale bridging mesoscopic polycrystal plasticity and nanoscale precipitation using a coupled full-field and mean-field strategy**

Safi, Ali Reza (1); Nanayakkara, Vimukthi (1); Chafle, Rupesh (1); Klusemann, Benjamin (1,2) 09:30
*1: Institute of Material and Process Design, Helmholtz Zentrum Hereon*
*2: Institute for Production Technology and Systems, Leuphana University Lüneburg*

The accurate prediction of microstructural evolution during thermo-mechanical processing of precipitation-hardened alloys requires capturing the complex interplay between plastic deformation and precipitation, a phenomenon known as dynamic ageing. In this regime, the accumulation of plastic strain, dislocation density, and excess vacancies modifies the nucleation, growth, and dissolution kinetics of secondary phases. However, modeling this coupling is computationally challenging due to the inherent separation of scales as precipitation processes operate at lengths smaller than the mesoscopic grains resolved by standard full-field models.

To address these challenges, this study establishes a unified computational framework for Al–Zn–Mg–Cu alloys that bridges the gap between mesoscopic grain evolution and nanoscale precipitation. A full-field crystal plasticity (CP) model, based on the multiphase-field (MPF) formalism [1], is coupled with a mean-field Kampmann-Wagner numerical (KWN) model [2]. The MPF model utilizes continuous order parameters to explicitly resolve grain boundary migration and recrystallization, ensuring stability under large deformations [3]. Simultaneously, the KWN module tracks the

strain-dependent evolution of $\eta'$ ($Mg_5Zn_7Al_6$) precipitates without requiring explicit spatial resolution. In this coupled scheme, local precipitate size distributions and volume fractions are derived from the thermo-mechanical history and dynamically influence the CP constitutive laws. The material model considers the contributions from precipitation, solid-solution, and work hardening to the critical resolved shear stress [4]. By linking these scales, the proposed framework can successfully capture the mutual dependencies between dynamic ageing, recrystallization kinetics, and the macroscopic mechanical response.

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**A Stochastic Finite-Strain Continuum Dislocation Dynamics Crystal Plasticity Model**

Lee, Sing-Huei (1,2); Schulz, Katrin (1,2)

*1: Karlsruhe Institute of Technology, Germany*
*2: Karlsruhe University of Applied Sciences , Germany*

09:50

Crystalline materials at small scales often show sample-to-sample scatter because plastic flow and hardening are governed by heterogeneous dislocation structures and crystallographic orientation. While uncertainty quantification in crystal plasticity has advanced, most studies treat randomness through local constitutive parameters or phenomenological hardening, and much less is known about how a spatially random initial dislocation field propagates when dislocations evolve by transport, curvature, and multiplication, especially in the presence of grain boundaries. Key open questions include the impact of the initial heterogeneity, which controls internal length scales, the impact of grain boundaries, which amplify variability through pile-ups and crystallographic discontinuities, and the impact of random initial conditions, which shape microstructure evolution and mechanical response. In this presentation, we develop a finite-strain dislocation-based crystal plasticity finite element framework coupled to continuum dislocation dynamics (CDD). The constitutive response is driven by CDD state variables and includes viscoplastic flow with nonlocal regularization; dislocation multiplication is modeled via a stress-dependent nucleation law. The finite-strain formulation provides a kinematically consistent treatment of lattice rotation and frame changes, and grain boundaries are modeled as impenetrable to dislocation transport to enable controlled study of dislocation pile-ups.
We apply the method by prescibing the initial total dislocation density as a spatial random field with controlled statistics and perform ensemble shear and tensile simulations for single crystals with a blocked boundary and for polycrystalline aggregates. We assess how initial microstructure randomness transfers to variability in mechanical response and near-boundary dislocation accumulation, and how these trends interact with intrinsic nonlocal length scales and source activation. Overall, the proposed finite-strain CDD crystal plasticity framework provides a kinematically consistent tool for studying stochastic material at microscale, and can be further use for uncertainty quantification in dislocation-transport-based crystal plasticity and for studying grain-boundary-controlled variability.

**Nonlocal strain gradient elasticity model for wave dispersion in materials at small scales**

Agiasofitou, Eleni; Lazar, Markus 10:10
*Technical University of Darmstadt, Institute for Mechanics, Germany*

In this study, the wave propagation behaviour in elastic media is presented within the framework of nonlocal simplified strain gradient elasticity theory [1]. This theory represents a unification of Eringen's nonlocal elasticity theory of Helmholtz type and the simplified first strain gradient elasticity theory and it is valid down to the Ångström-scale [2]. It incorporates two characteristic length scale parameters, namely the characteristic length $l_N$ of nonlocal elasticity of Helmholtz type [3] and the characteristic length $l_G$ of simplified first strain gradient elasticity.

The dispersion relations as well as the phase and group velocities for longitudinal and transverse acoustic waves are analytically determined [4]. A qualitative analysis of the phase and group velocities is also presented. It is found that nonlocal simplified strain gradient elasticity can exhibit normal or anomalous dispersion depending only on the values of the two characteristic lengths. Normal dispersion occurs when $l_N^2 > l_G^2$, whereas anomalous dispersion arises when $l_N^2 < l_G^2$. It is shown that in the case of normal dispersion, nonlocal simplified strain gradient elasticity yields physically realistic dispersive wave propagation in agreement with lattice dynamics. Moreover, a match between the obtained dispersion relations and those of the Born-von Kármán lattice model is established, leading to an important relation between the two characteristic length scales [4].

Nonlocal simplified strain gradient elasticity theory provides nonsingular solutions for all dislocation fields, it fulfils elastic stability and exhibits normal dispersion in agreement with lattice theory, thereby being an appropriate theory for the modelling of materials at small scales.

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## S06.2: Material modelling with non-metals

Organizer(s): Johlitz, Michael *(Universität der Bundeswehr München)*
Böhlke, Thomas *(Karlsruhe Institute of Technology (KIT))*

## S06.2.01: Material modelling with non-metals

Date: March 17, 2026 08:30–10:30
Room: KI, M11.82
Chair(s): Kehrer, Loredana
Böhlke, Thomas

### From Aggregated Mesostructure to Macroscopic Acoustic Performance: A Multi-physics Modeling for Silica Aerogels

Liu, Jie; Xiong, Weibo; Itskov, Mikhail 08:30
*RWTH Aachen, Germany*

Silica aerogels exhibit excellent sound absorption performance due to their highly complex, multiscale porous networks. However, establishing a physically interpretable link between their fractal structure and macroscopic acoustic behavior remains challenging. In this work, a bottom-up modeling framework is proposed to predict the normal incidence acoustic performance of silica aerogels by coupling mesoscopic diffusion-limited cluster aggregation (DLCA) simulations with continuum acoustic theory.

Three-dimensional aerogel structures are digitally reconstructed using the DLCA model, explicitly capturing their mass-fractal nature. Based on pore-size distributions exhibiting self-similar scaling and fractal theory, key transport parameters, specifically the pore space and tortuosity fractal dimensions, are extracted from the aggregation model. These dimensions allow for the analytical derivation of permeability and viscous/thermal characteristic lengths, eliminating the need for empirical corrections. These parameters are incorporated into the Johnson–Champoux–Allard (JCA)–Biot model to evaluate the effective sound absorption coefficient, while accounting for skeletal deformation. Numerical predictions show good agreement with experimental data for sub-millimeter silica aerogel particles, validating the framework ability to capture the acoustic signature, and paving the way for finite element simulations of complex shaped structures.

### Unique Determination of Elastic Material Parameters in Heterogeneous Materials using Mechanically Regularized Digital Volume Correlation and the Equilibrium Gap Method

Schmidt, Martin; Miska, Niklas; Balzani, Daniel 08:50
*Ruhr University Bochum, Germany*

Composite materials are widely used in mechanical engineering, construction, materials technology, and other fields since their material behavior can be well tuned to the specific demands of complex engineering applications. Thus, a suitable numerical model is required to predict the expected performance of such materials, which in turn necessitates the knowledge of appropriate material models in conjunction with their characterizing parameters for the individual phases of the composite. Therefore, the unique identification of those material parameters plays an important role, which is, however, not straightforward for parameters linked with an anisotropic or non-linear response. In this contribution, we present a new method for the determination of different elastic material parameters of individual phases of heterogeneous composite materials. This new method is based on the measurement of a three-dimensional displacement field and a subsequent computation of concerning material parameters by application of the equilibrium gap method (EGM). The displacement field is obtained from digital volume correlation (DVC) of measured CT images of the same specimen under different loading scenarios. Additionally, the DVC is enhanced by iteratively analyzing the DVC and the EGM, thereby mechanically regularizing the DVC-problem to ensure consistency of the computed displacement field with the mechanical problem. Since the discretized residual forces depend on the experimental boundary conditions, and the displacements are known from the DVC, the material parameters can be computed by solving an optimization problem aiming for minimized residual

forces. For parameters that appear linearly in the constitutive model, as will be the case for most elastic materials, the optimization problem will be quadratic and thus, a unique parameter identification can be achieved. As a further advantage of the EGM, this identification procedure is highly efficient since no solution of a nonlinear, discretized structural boundary value problem is needed, thanks to the full-field displacement data, provided that the mechanical boundary conditions are known. The proposed method is validated using a synthetically generated data set, which is obtained from a single CT image of an unloaded state. The associated deformed state is computed by artificial deformation of the CT picture by a deformation state obtained from a forward finite element computation. Since the real material parameters are known for this forward simulation, a qualitative evaluation of the results from the proposed method is enabled.

**Estimating the elastic properties of Bio-concrete using a constitutive model for cementation**

Wang, Yue; Nething, Christoph; Madadi, Hamid Reza; Eppinger, Erik; Class, Holger; Steeb, Holger; Blandini, Lucio
*University of Stuttgart, Germany*

09:10

Bio-concrete is a novel construction material in which biochemically induced calcite precipitation acts as a binder for sand particles, forming a load-bearing porous medium. Compared to conventional cement-based materials, this approach offers the potential for significantly reduced energy consumption during production. While existing numerical reactive transport models can successfully describe the temporal evolution of porosity and permeability during the bio-cementation process, a reliable estimation of the resulting elastic mechanical properties remains essential for practical applications and process design.

In this work, the porous medium is modelled as a two-solid-phase mixture consisting of sand grains and calcite cement. Inspired by natural cementation processes, a constant-cement constitutive model, originally developed in geomechanics to assess cementation effects in the underground rock formations, is adopted to describe the mechanical response of bio-concrete.

A series of laboratory experiments is conducted to produce bio-concrete specimens with different final porosities, enabling a systematic investigation of stiffness evolution as a function of porosity reduction. Both non-destructive and destructive tests (e.g. ultrasonic wave velocity measurements, unconfined compression tests, and chemical mass analysis) are performed to characterize porosity distribution and quantify the degree of cementation and the compressive strength. Based on the experimental data, the numerical model is calibrated and used to predict the mechanical properties, with the results compared against measurements. A Bayesian inverse modelling framework is then applied to quantify uncertainties arising from model assumptions and to identify key material parameters controlling the cementation-induced stiffness.

Lastly, the simulations are extended to the mesoscale, where spatial heterogeneities in the bio-cementation process are shown to influence the effective mechanical strength of the material.

**Automated constitutive modeling of dielectric elastomer actuators (DEAs)**

Amer, Gamal (1); Martonová, Denisa (2); Leyendecker, Sigrid (1)
*1: Institute of Applied Dynamics (LTD), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany*
*2: Institute of Applied Mechanics (LTM), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany*

09:30

Dielectric elastomer actuators (DEAs) enable muscle-like actuation by coupling finite mechanical deformations with strong electrical excitation, yet traditional constitutive modeling remains challenging because the mechanical response, electrostatic loading, and their coupling interact nonlinearly over wide operating ranges. Building on the concept of constitutive artificial neural networks (CANNs) [1], this work presents an automated, physics-informed model discovery strategy that learns an electromechanically-coupled Helmholtz free-energy potential $\psi$directly from data and obtains the nominal stress and electric displacement through differentiation, thereby enforcing thermodynamic

consistency by construction. Material frame indifference is embedded through invariant-based inputs spanning purely mechanical, purely electrical, and coupled electromechanical measures, while a sparsity-promoting identification mechanism selects the minimal set of relevant invariants and terms—so the entire functional form of the material model is discovered from data rather than simply calibrating coefficients of a priori imposed material model. In addition, the energy representation is constrained to avoid nonphysical responses (e.g. ensuring that $\psi$=0 in the undeformed, field-free configuration) and to promote stable extrapolation beyond the calibration set.

The proposed approach integrates the strengths of machine learning with the rigor of continuum physics. The trained model fits DEA's data across multiple loading conditions with high accuracy. To evaluate robustness and practical deployability, we introduce controlled noise perturbations (representing measurement uncertainty) and quantify the stability of the discovered energy form and derived predictions under increasing noise levels. The resulting constitutive law is also benchmarked against established electroelastic formulations to highlight the algorithm's generalizability and to clarify the learned model's discovered terms in an interpretable manner [2].

References:

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**Consistent time discretization of thermoelastic constitutive models based on physics-augmented neural networks**

Hartmann, Luis (1); Klein, Dominik (2); Franke, Marlon (1); Betsch, Peter (1) 09:50
*1: Karlsruhe Institute of Technology, Germany*
*2: TU Darmstadt, Germany*

In the present work a physics-augmented neural network is developed that serves as a thermomechanical constitutive model within a finite element code and fulfills relevant mechanical requirements of hyperelasticity by design.
For the consistent time discretization of the nonlinear material behavior, an energy–momentum scheme for dynamic simulations is proposed, which is specifically tailored to this constitutive model.
Synthetic data is used to train the neural network.
Various network architectures and calibration strategies are analyzed and compared.
Subsequently, both the neural network model and the conventional model are implemented into a finite element code.
In addition to the newly developed energy-momentum scheme, the classical midpoint discretization is implemented for comparison.
The more complex derivatives of the neural network compared to conventional models are explicitly taken into account.
The dynamic simulations show that the energy-momentum scheme is superior to the classical midpoint discretization in terms of numerical stability.
Furthermore, it is confirmed that the neural network is able to reliably learn and reproduce the behavior of the conventional constitutive model.
This demonstrates that neural networks are essentially nothing more than mathematical functions and can thus be used in numerical methods in the same way as conventional material models.

**Microscopic mechanisms and constitutive modeling of strain softening and hardening in glassy polymers**

Zhao, Wuyang 10:10
*FAU Erlangen-Nürnberg, Germany*

The large-deformation behavior of glassy polymers typically involves strain softening after yielding followed by strain hardening at larger strains. The microscopic processes underlying these regimes

and their representation in continuum models remain subjects of ongoing investigation. In this work, molecular dynamics simulations are employed to examine deformation mechanisms in glassy polymers under mechanical loading, with the goal of establishing connections between molecular-scale activity and macroscopic response.

Strain softening is explored by correlating local non-affine deformation with molecular rearrangements. Regions exhibiting pronounced non-affinity are found to be associated with increased bond-rotation activity, indicating an important role of configurational rearrangements during plastic deformation. These regions also display noticeable local volumetric fluctuations, which are spatially correlated with bond-rotation activity and may serve as a microscopic indicator of activated relaxation events. With increasing deformation, the spatial extent and intensity of these volumetric fluctuations increase around the yield strain, suggesting a transition from localized relaxation events to more collective structural rearrangements.

At larger strains, strain hardening is associated with heterogeneous stretching within entangled chain segments. Within each segment, a small subset of highly stretched bonds contributes significantly to the mechanical response. Averaging the stretch of these load-bearing bonds provides a measure of segmental deformation that evolves systematically with macroscopic strain and is consistent with rubber-like stress–strain behavior in the hardening regime. The influence of molecular parameters such as chain length, temperature, and strain rate on this response is briefly examined.

Based on these observations, a constitutive modeling framework is outlined that incorporates both segmental load-bearing deformation and stress-assisted structural relaxation. The resulting model captures key features of the stress–strain behavior of glassy polymers over a wide range of loading conditions and provides a physically motivated basis for describing strain softening and hardening in non-equilibrium polymer glasses.

## S06.2.02: Material modelling with non-metals

Date: March 17, 2026 16:30–18:30
Room: KI, M11.82
Chair(s): Johlitz, Michael
Böhlke, Thomas

### A comparative study of DCDC and SENB tests for Mode I fracture characterization of polymers

Diani, Julie; Coq, Arnaud 16:30
*Laboratoire de Mécanique des Solides, CNRS, Ecole Polytechnique, France*

An elastic and an elastoplastic methyl methacrylate polymer, both in the glassy state, were subjected to mode I fracture characterization using two different tests: the single edge notch bending (SENB) test and the double cleavage drilled compression (DCDC) test. The toughness of the elastic material was assessed using linear elastic fracture mechanics analysis. For the elastoplastic material, the J-integral was computed when strain fields were available.

Numerical analyses were performed using finite element simulations with two damage approaches: cohesive elements and phase-field modeling. This provided a comparison between the calculated J-integral and an estimate of the critical energy release rate when it could not be calculated otherwise. Both modeling approaches yielded similar results; however, the phase-field approach could not always predict the material toughness due to its dependence on the model regularization parameter.

For each material and each test, the estimated values of the critical energy release rate are in good agreement with the literature. More interestingly, for the same material, both tests provided significantly different estimates of this material parameter, leaving engineers uncertain about which test to choose for assessing material toughness in crack opening mode.

**Rate-Dependent Damage and Failure in Rubberlike Polymers: Characterization via a Gradient-Extended Thermomechanical Model at Finite Strains**

Bögershausen, Skadi (1); Kehls, Jannick (1); Reese, Stefanie (1,2); Scheunemann, Lisa (1); Brepols, Tim (1)

*1: Institute of Applied Mechanics, RWTH Aachen University, Germany*
*2: University of Siegen, Germany*

17:10

Silicone bonding is a key technology in the construction of glass façade systems, to name just one of many applications of polymers (see e.g. [1]). In such systems, the glass elements are bonded directly to the underlying support system. Constitutive models contribute to a deeper understanding of the highly complex mechanical behavior of polymeric materials, complementing traditional experimental investigations. Time-dependent and thermal effects have both been noted in the mechanical response of this type of material. Specifically, the accumulation of damage in these materials often depends strongly on loading rates, beyond the well-known viscoelastic behavior. The proposed constitutive framework captures these phenomena through a fully coupled thermomechanical formulation that takes large strains into account and combines viscoelasticity with a rate-dependent Perzyna-type damage formulation (see [2]). The material model incorporates a multiplicative decomposition of the deformation gradient into a thermal and a mechanical part, as well as into equilibrium and non-equilibrium parts. A gradient extension is added to regularize the damage field (see [3]). The model is able to describe damage caused by creep and relaxation. In order to determine the material parameters of a particular polymeric material based on experimental data, a staggered approach is used.

**Viscoelastic Modeling of Glacier Ice**

Sartorius, Jana (1); Humbert, Angelika (3); Steeb, Holger (1,2)

*1: Institute of Applied Mechanics (CE), Pfaffenwaldring 7, University of Stuttgart, 70569 Stuttgart, Germany*
*2: Stuttgart Center for Simulation Science, University of Stuttgart, Pfaffenwaldring 5a, 70569 Stuttgart,Germany*
*3: Alfred-Wegener-Institut Helmholtz Zentrum für Polar- und Meeresforschung, Germany*

17:30

The focus of this investigation is on the constitutive and numerical modeling of glacier ice under short-term stress variations, such as those caused by meltwater drainage events through fractures in large natural ice masses (Humbert et al., 2025). The aim is to realistically capture the viscoelastic behavior of polycrystalline ice during the primary creep phase. For this purpose, a three-dimensional generalised Maxwell model has been developed, in which volumetric deformations are assumed to be purely elastic, while isochoric deformations are modeled as viscoelastic. The material parameters are identified from creep data using a Prony series representation. The model is implemented using the open source finite element toolbox FEniCSx. To validate the characteristic rate-dependent deformation process, the numerical results are compared to time-harmonic (forced-oscillation) experimental compression tests. The results demonstrate that the proposed generalised Maxwell model, combined with the parameter identification approach, provides a solid foundation for the realistic simulation of deformable fractures in glacier ice.

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Humbert, A., Helm, V., Zeising, O., Neckel, N., Braun, M. H., Khan, S. A., Rückamp, M., Steeb, H., Sohn, J., Bohnen, M., and Müller, R.: Insights into supraglacial lake drainage dynamics: triangular fracture formation, reactivation and long-lasting englacial features, The Cryosphere, 19, 3009–3032, https://doi.org/10.5194/tc-19-3009-2025, 2025.

**Multiscale Characterization and Modeling of statistically inhomogeneous Moso Bamboo**

Speichinger, Lukas (1); Förster, Ralf (2); Böhlke, Thomas (1) 17:50

*1: Karlsruhe Institute of Technology (KIT), Germany*
*2: Berliner Hochschule für Technik (BHT), Germany*

Bamboo is considered the fastest-growing plant in the world and is distinguished by exceptional mechanical properties comparable to those of wood, making it an attractive material for sustainable construction. Its hierarchical structure results in significant anisotropy and spatial heterogeneity across the scales [1, 2], yet a comprehensive characterization and modeling of bamboo's mechanical behavior remains limited. While previous studies have investigated the mechanics of vascular bundles on the mesoscopic scale [3, 4] and bamboo's cellular structure on microsscopic scale [5, 6], a deeper understanding of the macroscopic behavior informed by multiscale structural features is still needed.

This contribution presents a computational approaches for characterizing and modeling the hierarchical structure and macroscopic linear elastic behavior of Moso bamboo (Phyllostachys edulis). Based on X-ray microtomography data [6] the cellular microstructure of bamboo is characterized, enabling the reconstruction of representative volume elements (RVEs) via advanced tessellation algorithms. The effective behavior of the cellular structure is computed by FFT-based homogenization.

The statistically inhomogeneous mesostructure of the culm wall is characterized via advanced computational image processing techniques, including the segmentation of cross-sectional images, AI-driven identification of individual vascular bundles, and Torquato-based statistical analysis to extract structural characteristics. According to the measured characteristics a RVE of the mesostructure can be reconstructed for any radial position within the culm wall. The generated RVE reflects the structural characteristics of a given radial position without considering the gradient of the characteristics and therefore is statistically homogeneous. Again FFT-based homogenization is applied to the mesostructural RVEs incorporating the effective cellular properties.

The proposed approach enables systematic investigation of bamboo's anisotropy and heterogeneity, bridging microscopic and mesoscopic phenomena to inform macroscopic behavior. This multiscale modeling framework provides fundamental insights into structure-property relationships in bamboo and establishes a basis for predictive simulations supporting its application in sustainable structural design.

References:

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**Fractional Modeling of Moisture-Dependent Viscoelastic Behavior in Thermoplastic Polymers**

Fauser, Dominik (1,2); Beddrich, Jonas (3); Wohlmuth, Barbara (3); Steeb, Holger (1,2) 18:10

*1: Institute of Applied Mechanics (CE), University of Stuttgart, Pfaffenwaldring 7, Stuttgart, D-70 569, Germany*

*2: Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Pfaffenwaldring 5a, Stuttgart, D-70 569, Germany*

*3: Department of Mathematics SoCIT, Technical University of Munich, Boltzmannstraße 3, Garching, D-85 748, Germany*

The viscoelastic response of thermoplastic polymers is strongly affected by environmental conditions, particularly temperature and moisture. Elevated temperatures enhance chain mobility and reduce stiffness, while absorbed moisture acts as a plasticizer and leads to pronounced changes in thermo-mechanical properties within the glass transition range. Although the time-temperature superposition principle effectively characterizes the behavior of thermo-rheologically simple materials, an analogous framework for moisture-dependent effects remains underdeveloped.

In this contribution, we present a continuous description of the thermo-viscoelastic behavior of thermoplastic polymers under simultaneously varying temperature and moisture levels. Fractional viscoelastic models are employed due to their compact parametrization and their ability to capture the characteristic asymptotic behavior of the loss factor, which standard discrete rheological models often fail to reproduce. The proposed approach is validated using a newly generated data set that systematically resolves moisture-induced changes in the mechanical response. Its predictive capability is benchmarked against the generalized Maxwell model.

The results show that the fractional formulation robustly captures moisture-dependent thermo-viscoelasticity while requiring significantly fewer parameters than classical rheological models, offering a promising framework for efficient and accurate material modeling under coupled environmental conditions.

## S06.2.03: Material modelling with non-metals

Date: March 18, 2026 16:30–18:30
Room: KI, M11.82
Chair(s): Juhre, Daniel
Böhlke, Thomas
Johlitz, Michael

**Modelling functionally graded 4D Printing Materials**

Hembrock, Henrik (1); Andrae, Heiko (1); Müller, Ralf (2); Pretsch, Thorsten (3); Galambos, Theodor (3); Temme, Kerim (3); Chalissery, Dillip (3) 16:30

*1: Fraunhofer ITWM, Germany*

*2: TU Darmstadt*

*3: Fraunhofer IAP, Germany*

Functionally graded materials (FGMs) have gained increasing attention in recent years due to their unique ability to exhibit spatially varying properties. Applications range from rapid disassembly to patient-specific, self-deploying medical devices. One promising manufacturing approach is 4D printing, which utilizes shape memory polymers (SMPs) printed with fused filament fabrication (FFF). By locally programming material behavior through printer settings – such as nozzle temperature and print speed – complex shape changes can be achieved.

While numerous experimental studies have investigated the shape-changing behavior of 4D printed structures, there is a lack of physical models that enable predictive simulations. Consequently, optimizing printer parameters to achieve a desired deformation remains an open challenge.

A new numerical process simulation for FFF of SMPs is proposed, taking into account process parameters such as temperature, printing speed, and print paths. This approach involves parsing GCode for

simulation input and incorporating a physical model of decay effects caused by reheating during successive layer deposition. By applying laminate theory, the layer-wise strain mismatch responsible for 4D printed beams is leveraged to experimentally identify key physical parameters without requiring a full thermo-mechanical simulation of the build process.

Future research will extend this framework to develop an inverse shape optimization model for 4D printed structures. This will enable direct determination of target parameters – such as temperature and printer speed – closing the loop between machine code and simulation for precise control of shape programming.

Chalissery, Dillip et. al; Highly Shrinkable Objects as Obtained from 4D Printing, Macromolecular Materials and Engineering 2021

**Numerical Modeling and Experimental Full-Field Validation of Non-Planar 3D-Printed Components**

Ewougsi Tekeu, Christian-Lionel; Tröger, Jendrik-Alexander; Afshari, Arash; Inkermann, David; Hartmann, Stefan
*Clausthal University of Technology, Germany*

16:50

Conversely to traditional planar 3D-printing, non-planar 3D-printing techniques have emerged in the field of additive manufacturing. Several works reveal that – compared to planar 3D-printing – components manufactured by non-planar techniques depict exceptional mechanical properties as a result of material alignment in all spatial directions, thereby, allowing for load-oriented material deposition.

Non-planar printing requires optimal print trajectories, which demand the integration of accurate, flexible numerical simulations. These simulations are vital for refining the printing path, and for topology optimization of the 3D-printed components. Despite its importance, the anisotropy caused by the layering process is frequently ignored, especially when linear elastic material behavior is assumed in the numerical simulations. This might lead to significant model errors.

To bridge these limitations, we introduce a novel flexible modeling approach for both planar and non-planar 3D-printed components by using finite element simulations based on G-code data. We employ continuous interpolation of G-code data to determine the spatially varying preferred directions of anisotropy required for modeling.
Moreover, we draw on full-field measurements by means of stereo-correlation-based digital image correlation to validate our numerical simulations. Due to the commonly non-flat geometry of non-planar components, experimental validation becomes challenging, as the geometry alignment inherently leads to mixed loading scenarios. However, this work reveals that digital image correlation provides more reliable results when displacement fields on non-flat surfaces are evaluated, compared to traditional force-displacement data.

**Viscoplastic modeling of shotcrete 3D printing material**

La, Quoc Tuan (1); Meyer, Knut Andreas (2); Kollmannsberger, Stefan (3); Jänicke, Ralf (1)
*1: Technische Universität Braunschweig, Germany*
*2: Chalmers University of Technology, Sweden*
*3: Bauhaus-Universität Weimar, Germany*

17:10

In recent years, Additive Manufacturing in Construction (AMC) has provided an alternative method for the building industry by offering a faster and more efficient way to build with concrete. Unlike traditional methods that rely on molds, AMC deposits material layer by layer, enabling new possibilities for custom designs and complex shapes. AMC also digitalizes the construction process, which helps reduce labor costs, cut material waste, and streamline the transition from design to construction. To fully optimize these advantages, AMC requires appropriate modeling of building components and deposition processes.

Many developments have focused on digital methods for designing parts and planning AMC processes [1], while others have provided numerical simulations to predict the failures of AMC structures [2].

Our study contributes to the latter, aiming to develop a modeling and simulation approach for bulk-deposited AMC concrete and its interlayers. From this, a homogenized substitute model is developed to reduce the computational cost of simulating complex geometries on a part-scale.

This contribution develops a thermodynamically consistent viscoplastic model for shotcrete 3D printing material. The model is based on Perzyna's viscoplasticity and incorporates Bingham-type rheology to represent the thixotropic behavior of freshly printed shotcrete. Additionally, the mechanical properties evolve depending on internal microstructural build-up processes and the actual plastic deformation rate acting on the material. Finally, the thermodynamic consistency of the model is demonstrated and numerical results are presented.

**References**:

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**Phase field crystal model of out-of-plane deformations in thin crystalline sheets induced by thermal expansion**

Radice, Emma (1); Salvalaglio, Marco (1,2); Voigt, Axel (1) 17:30
*1: Institut für Wissenschaftliches Rechnen, TU Dresden, Dresden, Germany*
*2: Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany*

Thin, flexible crystalline sheets exhibit unique elastic properties due to their ability to undergo out-of-plane deformations. Understanding this behavior requires a description that couples in-plane elasticity, out-of-plane bending and the presence of defects.
We develop a mesoscale description for these systems by extending the Phase-Field Crystal (PFC) model. The PFC model describes crystal structures at diffusive timescales through a periodic, microscopic density field and it allows one to incorporate both elasticity and topological defects into a continuum description. In comparison to previous approaches, our extension permits a spatially varying equilibrium lattice spacing, enabling the representation of localized lattice eigenstrain to mimic thermal effects or lattice mismatch in heterostructures.
We validate the extended model against analytical predictions from the Föppl–von Kármán equations for uniaxial compression and from Eshelby's inclusion problem. Using this validated framework, we then study how locally induced compressive stresses drive out-of-plane deformation in the sheets.
Our approach, implemented via a Fourier pseudo-spectral method, exploits the PFC model's natural ability to capture the complex, coupled interactions among elasticity, out-of-plane bending and defect dynamics.

**About the complex Poisson's ratio in linear viscoelasticity**

Steeb, Holger 17:50
*University of Stuttgart, Germany*

Within the framework of uniaxial time-harmonic experiments, the complex Poisson's ratio, together with the complex elastic modulus, uniquely characterizes the transient behavior of an isotropic linear viscoelastic material. From an experimental point of view, the complex Poisson's ratio can be determined directly from the amplitudes and phase shifts of axial and longitudinal strains. In contrast to the complex elastic modulus, or more generally to all moduli, no additional force quantities (or subsequently determined stresses) need to be measured for the Poisson's ratio.

Despite the straightforward interpretation of the complex Poisson's ratio, there has been considerable debate in the literature regarding its (theoretical) definition and its measurability, with frequent—yet often incorrect—analogies being drawn to complex moduli and compliances.

In this contribution, we experimentally investigated cylindrical samples of polymethylmethacrylate (PMMA) and Berea sandstone using different measurement setups to compare the two methods for different materials. For direct measurements, strain gauges were used in harmonic uniaxial tension and compression tests to measure longitudinal and transverse strains.

Our experimental results confirmed that the loss factor of the complex Poisson's ratio can be either positive or negative (for PMMA and sandstone), depending on which strain lags more behind the axial force excitation, in agreement with theoretical expectations.

**Mullins softening with neural network constitutive models**
Klein, Dominik K.; Fey, Jonas; Kannapinn, Maximilian; Weeger, Oliver
*TU Darmstadt, Germany*
18:10

We formulate physics-augmented neural network (PANN)-based constitutive models for Mullins softening material behavior. This enables the constitutive modeling of soft rubbers, polymers, composites and metamaterials with stress-softening or damage in cyclic loading. The pseudo-elastic approach [1] is based on an isotropic hyperelastic PANN model [2] which is complemented by a damage function to model softening. The damage function is based on feed-forward neural networks, for which we investigate the influence of different monotonicity and convexity constraints. We furthermore consider parametric dependencies of the material behavior. With this PANN architecture, a physically sound behavior of the damage factor and the thermodynamic consistency of the model are ensured. We apply the PANN model to multiaxial, cyclic experimental data of an EPDM material synthesised with different amounts of sulphur contents [3] The PANN model shows an excellent performance both in representing the ground truth material behavior and in nonlinear finite element analysis.

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## S06.2.04: Material modelling with non-metals

Date: March 19, 2026 08:30–10:30
Room: KI, M11.82
Chair(s): Böhlke, Thomas
Johlitz, Michael

**Temperature-related phenomena in polymers**
Lion, Alexander; Johlitz, Michael
*Universität der Bundeswehr München, Germany*
08:30

Compared with metals, the characteristic temperatures at which polymers change their behaviour are smaller. Temperature-related phenomena in meltable thermoplastics, weakly crosslinked elastomers or highly crosslinked thermosets have their origin in physical or chemical alterations on the microscale. On the macroscopic scale, the mechanical, thermal and caloric properties of polymers change. Some of these phenomena are reversible, but others are irreversible. They take place when the temperature is changing due to external heat supply or inelastic energy dissipation caused by dynamic mechanical loads. As we know, growing temperature increases the mobility of the polymer molecules and changes the rates of chemical reactions. This talk addresses selected phenomena that are relevant for technical applications. As a reversible phenomenon, the behaviour of polymers around the glass transition is treated. Crystallisation, driven by deformation or temperature, is also a reversible phenomenon of interest. Adhesives change their properties during curing in an irreversible manner. Another phenomenon of high technical importance is ageing. Irreversible chemical ageing

increases with the temperature or the environmental oxygen concentration. It results from the generation of new crosslinks in combination with chain scission and modifies the mechanical material behaviour. Another characteristic phenomenon, especially of thermoplastics, is physical ageing. It occurs below the glass transition, is thermoreversible, corresponds to a decrease in the free volume and leads to an increase in the relaxation times. If polymer parts are cyclically deformed over long times, dissipative heating takes place and leads to an increase in temperature. The focus of this talk is material modelling. Experimental data support the argumentation.

**Mechanical preconditioning and its implications for material modeling**

Wollner, Maximilian P. (1); Holzapfel, Gerhard A. (1,2) 09:10
*1: Graz University of Technology, Austria*
*2: Norwegian University of Science and Technology, Norway*

The mechanical behavior of a wide range of polymers and soft biological tissues is characterized by a damage mechanism referred to as the Mullins effect. From an idealized point of view, these materials exhibit an initial stress response upon primary loading, which is then permanently softened in unloading and reloading until the previous maximum level of loading is exceeded again [1].

Several constitutive models have been proposed for the description of the Mullins effect [2,3]. It is nonetheless common to disregard this type of softening based on the observation that repeated cycling leads to stable material behavior, i.e., additional cycles do not significantly alter the stress trajectory [4,5]. In many works, a constitutive model is then fitted to this stable but damaged material response without explicitly resolving the Mullins effect. For such a simplification to hold, the following is tacitly assumed: the maximum loading that a material point experiences during a general deformation is comparable to the maximum loading in the experiements used for calibration.

In this contribution, we investigate the validity of the aforementioned assumption. To this end, we calibrate two distinct material models to the same set of experimental data. One model explicitly resolves softening and is therefore calibrated to the entire data set. The other model is only fitted to a single unloading and reloading cycle, neglecting primary loading and the Mullins effect. We then compare the predictions of both material models in a boundary-value problem not previously used for calibration. The subsequent discussion of the results highlights the interplay between theory and experiment.

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**Modelling the viscoelastic behaviour of Alginate-Gelatine Hydrogels**

Graham, Marc (1); Klinge, Sandra (1); Kurreck, Jens (2) 09:30

*1: Department of Structural and Computational Mechanics, TU Berlin, Germany*
*2: Department of Applied Biochemistry, TU Berlin, Gustav-Meyer-Allee 25, 13355 Berlin*

Hydrogels are widely being used in cell-culture to provide a scaffolding medium, allowing cells to grow in a 3D environment. Typically, 3D-printing is used to layer the different cell-types and to produce structures such as perfusions that lead to miniaturised models of human organs [1], e.g. lungs, livers, intestines.
The application has a fundamentally mechanical nature since: a) printing through a small nozzle induces viscous forces and can kill the cells prematurely; b) viscosity allows better control of the structure geometry and the structures themselves can be subjected to internal pressure loading; and c) the viscoelastic properties of the hydrogel are known to determine cell survival rate in the culture and the establishment of a functioning extracellular matrix [2].

Cyclically-loaded samples of alginate-gelatine hydrogels under indentation show that the material responds viscoelastically, including relaxation and internal friction, similar to many polymers. The material is very compliant and undergoes large deformations at even very moderate loads.

Presented is a homogeneous, objective, finite-strain material model inspired by the microstructure, as observed under electron microscope. The contact problem of the indentation ball is solved by the recently-published Latent Variable Proximal Point algorithm [3]. Finite element discretisation using the FEniCS library allows the model to be parameterised to reproduce the experimentally-observed material responses.

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**Impact of Additives and Preconditioning on Thermal and Thermoviscoelastic Behavior of Thermoplastics**

Huang, Yiheng (1,2); Kehrer, Loredana (2); Reinhardt, Eike (1); Burbulla, Frank (1); Böhlke, Thomas (2) 09:50

*1: Dr. Ing. h.c. F. Porsche AG, , Germany*
*2: Institute of Engineering Mechanics, Continuum Mechanics (ITM-KM), Karlsruhe Institute of Technology (KIT), Germany*

Advanced material models for crash analysis rely on high-quality experimental data that resolve the thermomechanical response across relevant time and temperature scales. The present study provides such data, forming a robust basis for improved constitutive modeling for polypropylene components.

The thermomechanical behavior of polypropylene was systematically investigated to support the calibration and validation of advanced constitutive models. This work thus focuses on polypropylene, a representative thermoplastic whose long-term performance is strongly governed by thermal history [1], while post-crystallization effects and associated changes in viscoelastic properties are often neglected in engineering practice. The study examines the influence of thermal preconditioning, aging, and talc reinforcement on post-crystallization behavior, thermal expansion, and viscoelastic properties.

Therefore, neat and talc filled samples are investigated in three material states, namely unconditioned, thermally preconditioned, and aged. Thermal expansion is measured by dilatometry and viscoelastic behavior is characterized by dynamic mechanical analysis over identical temperature windows and broad frequency ranges. Unconditioned polypropylene shows pronounced post crystallization during heating, whereas preconditioned samples exhibit nearly stable dimensions and aging partly reactivates structural rearrangements [2]. Talc reinforcement reduces thermal expansion by restricting molecular mobility. The dynamic mechanical analysis reveals a glass transition in the amorphous phase and a high temperature $\alpha$*-relaxation associated with interactions between crystalline and amorphous regions [3].

The results demonstrate how thermal history, filler content, and aging govern relaxation processes and stiffness evolution in polypropylene and provide an experimental basis for improved processing strategies and more reliable long-term performance predictions.

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**When Invariants Matter: The Role of I1 and I2 in Neural Network Models of Incompressible Hyperelasticity**

Dammass, Franz; Kalina, Karl A.; Friedrichs, Konrad; Kästner, Markus 10:10
*TU Dresden, Germany*

Physics-augmented neural networks (PANNs) provide a framework for flexible and accurate constitutive modelling. For the formulation of these models, the usage of invariants of deformation tensors is attractive, since this can a priori guarantee objectivity and material symmetry. In this work, we focus on incompressible, isotropic hyperelasticity and consider our recently proposed polyconvex invariant-based PANN that enables the isochoric-volumetric split of the free energy [1, 2].

In this contribution, we aim at enhancing the understanding of deformation invariants. We discuss the set of invariants that are actually admissible, i.e., for which (I1, I2) a physical deformation state does indeed exist. Furthermore, we prove that uniaxial and equi-biaxial deformation states correspond to the boundary of the set of admissible invariants. Moreover, we study how the experimentally-observed constitutive behaviour of different materials can be captured by means of neural network models of incompressible hyperelasticity, depending on whether both I1 and I2 or only one of the two, i.e., either solely I1 or only I2, are taken into account. To this end, we investigate three different experimental data sets from the literature.

In addition, we give a short outlook on the hybrid modelling of fracture, combining the PANN with the classical phase-field approach to fracture [2], and on the PANN modelling of strain-induced crystallisation in rubber [3].

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## S06.2.05: Material modelling with non-metals

Date: March 19, 2026 17:30–18:50
Room: KI, M11.82
Chair(s): Wollner, Maximilian Peter
Johlitz, Michael

### Finite-strain material modeling and inverse parameter identification of swelling-induced deformations in hydrogels

Rinke, Felix (1); Steeb, Holger (1,2) 17:30
*1: University of Stuttgart, Institute of Applied Mechanics (MIB), Pfaffenwaldring 7, D-70569, Germany*
*2: University of Stuttgart, Stuttgart Center for Simulation Science (SC SimTech), Pfaffenwaldring 5a, D-70569 Stuttgart*

Hydrogels exhibit large, stimuli-induced volumetric deformations and are therefore of potential interest for applications in soft robotics, e.g. in bilayer or multilayer devices. The total deformation of hydrogels arises from the coupling of mechanical effects and diffusion-driven swelling, posing challenges for constitutive modeling within a consistent continuum mechanical framework.

In this contribution, we present a finite-strain formulation for hydrogels based on a multiplicative decomposition of the deformation gradient into mechanical and swelling-induced components. Input data for model calibration, representing the coupled mechanical and swelling-induced response at finite strains, are employed within this framework. The methodology enables systematic separation of the underlying deformation mechanisms, allowing inverse identification of the associated model parameters.

The proposed approach is implemented in the open-source finite element solver CalculiX and demonstrated on hydrogel-based actuators as representative applications. The results highlight that a fully nonlinear finite-strain description is essential to accurately capture the volumetric response of hydrogels at large swelling ratios.

Future work will extend the framework to transient problems, with particular emphasis on differing diffusion time scales and their influence on swelling-induced deformation processes.

### Humidity and UV Effects on PA 6 Thermoviscoelasticity

Kehrer, Loredana (1); Hirschberg, Valerian (2); Keursten, Johannes (1); Böhlke, Thomas (1) 17:50
*1: Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*
*2: Technical University Clausthal, Clausthal-Zellerfeld, Germany*

Polyamide 6 (PA 6) components are often subjected to varying climate conditions, including humidity [1,2] and ultraviolet (UV) radiation [3], which can impact stiffness, damping, and long-term performance. To separate and quantify these influences, this study investigates (i) the effects of hydrothermal treatment on linear viscoelasticity and (ii) UV-driven aging mechanisms on moisture-equilibrated materials using a consistent dynamic mechanical and multi-scale characterization strategy.
In the hydrothermal study, PA 6 is investigated for distinct conditioning states, ranging from dry-as-molded to standard atmosphere and fully water-saturated specimens. Dynamic mechanical analysis (DMA) was performed using relaxation and temperature-frequency sweep tests under both controlled and non-controlled humidity conditions in order to capture intrinsic, moisture-induced softening as well as test-induced responses.
In the UV-aging study, moisture-equilibrated PA 6 is exposed to controlled short- and long-term UV irradiation. Gel permeation chromatography (GPC), differential scanning calorimetry (DSC), and DMA were used to correlate molecular changes, thermal state, and thermoviscoelastic response. Early UV exposure results in distinct stiffening despite only marginal variations in molar mass and crystallinity. Prolonged irradiation results in progressive molar mass reduction, indicating ongoing chain scission.

This is accompanied by a loss of stiffness and an increase in viscoelastic dissipation. Temperature-frequency sweeps and master curve construction show that UV exposure alters the relaxation spectrum and reduces the applicability range of time-temperature superposition.

References:

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**An anisotropic hyperelastic-plastic material model considering process-structure-property relations for injection moulded thermoplastic vulcanisates**

Mentges, Noah; Çelik, Hakan; Dahlmann, Rainer; Hopmann, Christian 18:10
*Institut für Kunststoffverarbeitung an der RWTH Aachen, Germany*

Integrative simulation chains for injection moulded plastic components combine initial process simulations with structural calculations of the components. Thereby, process-dependent microstructural information is mapped to the FE-mesh to be considered in the constitutive model of the solver. In many structural plastic applications, this method is already state of the art, for improved anisotropic mechanical response and strength predictions.

Thermoplastic elastomers and especially thermoplastic vulcanisates (TPV) pose significant process-dependent anisotropic mechanical responses due to orientation processes of the phase configuration during injection moulding. TPV consist primarily of a discontinuous, vulcanised elastomeric phase and a continuous thermoplastic phase. Due to this multiphase structure, thermoplastic vulcanizates (TPV) combine rubber-elastic properties of elastomers with the processability and recyclability of thermoplastics. Due to the flow and cooling conditions in injection moulding, elastomer particles are oriented and stretched within the direction of flow. The process conditions fixate the elastomer particles in the stretched state, resulting in a preferential material direction. Under quasi-static uniaxial loading, anisotropy can result in a reduction of stress response of up to 40 % in dependence on the testing direction with respect to the flow direction.

Modelling the particle deformation behaviour in injection moulding simulation is not trivial due to viscoelastic processes during the injection and cooling phase. However, qualitative solutions to this already exist. Existing constitutive mechanical models for TPV, however, cannot consider the local process- and morphology-related anisotropy. To account for this, in this work, an analytical anisotropic, elastic-plastic material model is presented, which gives an accurate prediction of the material behavior given the local phase configuration. The model is based on a semi-physical homogenisation approach on the molecular level. It uses a full-network hyperelastic modelling framework. By implementing rheological frameworks in microscopic stress formulation, it can consider micromechanical phase interactions of different regions of the microstructure, including plastic deformation and stress softening. Anisotropy is considered by imposing an orientation distribution on the network model in relation to the deformation state of the elastomer particles.

The presented model is investigated analytically and compared to mechanical investigations using specimen simulations. It can represent the characteristic phenomena of macroscopic testing under tensile loading. Current simulations are related to measured particle deformation in microscopic investigations. In future work, quantitative prediction methods for the process-dependent local orientation state must be developed for a fully coupled integrative simulation chain for TPV.

**Investigating Subglacial Cavity Evolution Using Two-Dimensional Viscoelastic Ice Sheet Modeling**

Heck, Luisa (1); Spreng, Jonas (1); Lemire, Annie (2); Vasen, Mariette (4,5); von Dobschütz, Henriette (3); Schubert, Martha (3)

*1: Ruprecht-Karls-University, Heidelberg, Germany*
*2: University Bremen, Bremen, Germany*
*3: Friedrich-Schiller-University Jena, Jena, Germany*
*4: Karlsruhe Institute of Technology, Karlsruhe, Germany*
*5: University of Oxford, Oxford, UK*

18:30

Ice sheets are complex dynamic systems whose flow is strongly influenced by subglacial hydrology and bedrock topography. This study aims to improve the understanding of the interaction between water-filled subglacial cavities and the overlying ice sheet by investigating their coupled behaviour. This is achieved by simulating a two-dimensional cross-section of an ice sheet using a nonlinear viscoelastic Maxwell material model. The nonlinearity in the viscosity is considered by Glen's flow law. The temperature dependency of the viscosity is incorporated by assuming a depth-dependent temperature profile. Motivated by radar measurements, we simulate a representative ice-sheet cross section consisting of a 5 m long, 1 m high cavity embedded within a 1000 m high, 2000 m long ice domain. Cavity evolution is then modeled using FEniCSx, a Finite Element Method framework. To resolve regions with high gradients in the fields, an unstructured mesh with local refinement around the cavity and the lower and upper boundary of the cross-section is used. The main objective of this study is to quantify the change in cavity area in response to variations in water pressure and ice velocity. A parameter study covers water pressures from 1 MPa to 20 MPa and ice velocities between 0.0 m/day and 1.0 m/day, with a total simulation time of 25 days. This range captures both the shrinking and growth of the cavity. The results provide a basis for improving representations of cavity dynamics in ice sheet models.

## S06.2.06: Material modelling with non-metals

Date: March 20, 2026 08:30–10:30
Room: KI, M11.82
Chair(s): Lion, Alexander
Böhlke, Thomas

**Digital twinning of thermoplastic pellets extrusion process**

Soares da Silva, Elder (1); Brousse, Clément (3); Jabir, Mouad (2); Bouchonneau da Silva, Nadège (2); Jochum, Christian (1); Radford, Don W. (3)

*1: ENSTA, France*
*2: Federal University of Pernambuco (UFPE), Brazil*
*3: Colorado state University, Fort-Collins CO, USA*

08:30

Extrusion of pellets for processing thermoplastic parts is gaining increasing attention as a sustainable alternative to thermosets and a promising material for 3D printing applications. However mechanical properties obtained are highly process dependent and require a detailed understanding of the thermal and rheological state of the polymer. This work presents a three-dimensional finite element modeling approach of PET-G pellets during the extrusion process for 3D printing developed at ENSTA Brest Campus and implemented in COMSOL Multiphysics [1-2]. This is a collaborative work with Colorado State University in charge of the design of a 3D printing device based on a Dyze Design industrial extruder.

The modeling approach couples creeping-flow Stokes equations with heat transfer in fluids, using temperature- dependent laws for viscosity, density and thermal properties of the polymer. Since it is an inelastic non-Newtonian fluid, viscosity depends on the shear rate and temperature. To address this fact, two different models were used: Power Law [3] and Cross [4-6], in order to compare the performance of the solutions between the approaches. A Frozen Rotor formulation [2] captures the shear-driven motion generated by the screw while keeping the computational cost tractable. The

detailed representation of the screw, barrel, and die enable the model to resolve thermal gradients and the helical flow patterns characteristic of single-screw extrusion.

Simulations demonstrate complete polymer melting within the designed heating zones, with peak temperatures ranging from 220 °C to 240°C - consistent with PET-G's processing window. Beyond reproducing the thermal and flow physics, the model provides a practical framework to control outlet mass flow rate by adjusting boundary conditions such as heating-zone temperatures (three independent zones) and rotational speed of the screw, as well as geometric parameters, especially the nozzle diameter, offering a pathway toward optimized extrusion performance and the scaling up of the process.

This initial study of single-screw extrusion proved to be quite effective, producing mass flow rate predictions with a margin of error of around 5% in relation to experimental measurements. A proposal for porosity development, based on density evolution during the process, is presented and highlights the importance of pellets initial moisture content on mass flow rate.

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**Viscoelastic Material models in the context of Digital twins**

Budihala, Gajendra Babu 08:50
*Ulm Univerisity, Germany*

The rapid advancement of Industrial technologies and data collection and handling methods has paved the way for the widespread adoption of **Digital Twins (DTs)** in engineering, enabling seamless integration between physical systems and their virtual counterparts. Digital Twins are dynamic, real-time digital replicas of physical assets, systems, or processes designed to optimise performance, enhance predictive capabilities, and support decision-making across diverse engineering domains.

The current work presents a comprehensive framework for building robust and scalable Digital Twins tailored for material testing applications using a universal testing machine (UTM), focusing on core challenges such as material modelling, model fidelity, data integration, and computational efficiency. Our goal is to build a Digital Twin of a polymer material subjected to cyclic loading. A linear viscoelastic material model with its governing PDE is considered in this case. The model is used to simulate the material's behaviour through the finite element method. In this work, energy-based methods for fatigue life prediction are incorporated. Later, the high-fidelity solution obtained is reduced using a reduction basis (RB) method, which improves computational efficiency.

Our approach integrates physical knowledge, which is available in terms of constitutive or material modelling, and real-time sensor data to construct and continuously update the Digital Twins. Emphasis is placed on the knowledge available through Partial Differential Equations, which address the reliability and robustness of the digital twin model. This work highlights the advantages of digital twins in the predictive maintenance and health monitoring of assets or systems, which eliminates unexpected failures and downtimes in engineering applications.

**A finite viscoelastic Maxwell model for ice shelves using an exponential update and Glen's flow law**

Koßler, Marvin (1); Müller, Ralf (2); Humbert, Angelika (3,4); Schröder, Jörg (1) 09:10
*1: University of Duisburg-Essen, Germany*
*2: TU Darmstadt, Germany*
*3: Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Germany*
*4: University of Bremen, Germany*

In the context of rapidly diminishing polar ice masses, the modeling of ice shelves is of critical importance. An adequate description of ice shelf dynamics requires the ability to capture both short-term elastic responses and long-term viscous flow, particularly under changing loading conditions, see [1].

This contribution presents a finite viscoelastic Maxwell model for ice that consistently accounts for both short-term and long-term deformations, see [2]. The formulation is based on a multiplicative decomposition of the deformation gradient into elastic and viscous parts and is derived using a Lie derivative. An exponential update scheme, see [3], is employed for the time integration of the internal viscous variables, ensuring an inherently isochoric viscous flow over long simulation times.

To represent the nonlinear creep behavior of ice, the classical Maxwell model is extended by incorporating Glen's flow law, see e.g. [4], resulting in a stress-dependent effective viscosity. This extension allows for a coupling between effective stress levels and viscous flow while preserving the structure of the exponential integration scheme.

The performance of the proposed model is demonstrated using ice shelf benchmark problems of which the numerical results are presented in terms of stress and displacement evolution.

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**Modeling Mechanical and Caloric Relaxation Processes in the Glass Transition Regime of Polymeric Materials**

Hille, Frederik (1); Keursten, Johannes (1); Enders, Sabine (2); Böhlke, Thomas (1) 09:30
*1: Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Germany*
*2: Institute of Technical Thermodynamics and Refrigeration, Karlsruhe Institute of Technology (KIT), Germany*

Polymeric materials are known to have a distinct glass transition regime in which mechanical and caloric properties, such as the stiffness and the heat capacity, change significantly with the temperature [1]. This behavior also manifests in substantial relaxation processes for both the stresses and the enthalpy within this regime. Additionally, these processes are coupled with each other, e.g., due to self heating caused by viscoelastic dissipation effects. Therefore, taking both relaxation processes into account simultaneously helps to gain additional insight into the material behavior of polymeric materials.

In this talk, we present a short overview of existing state-of-the-art thermodynamic frameworks used to describe viscoelastic material behavior, see, e.g., [2], [3], as well as caloric relaxation processes, see, e.g., [4], [5]. We then focus on a combined model considering both effects in a unified framework by reformulating the model of Keursten et al. [6], which is based on an internal variable approach by Lion et al. [4]. This allows us to further exploit the analogy between mechanical and caloric relaxation effects within the glass transition regime, as well as to efficiently investigate the thermodynamic consistency of the used model. Additionally, the model can be directly extended to incorporate energetic and dissipative nonlinear effects within the different relaxation processes.

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## S07: Coupled problems

Organizer(s): Düster, Alexander *(Hamburg University of Technology)*
Kästner, Markus *(TU Dresden)*

## S07.01: Coupling strategies

Date: March 17, 2026 08:30–10:30
Room: KII, M17.02
Chair(s): Düster, Alexander
Kästner, Markus

### Partitioned Coupling for Multi-Field Problems – from Muscles to Subsurface

Schulte, Miriam; Chen, Jun; Chourdakis, Gerasimos; Homs Pons, Carme; Desai, Ishaan; Schneider, David; Simonis, Frederic; Uekermann, Benjamin
*University of Stuttgart, Germany*

08:30

Partitioned coupling for multi-field problems is based on the idea to 'simply' se existing solvers for each of the involved fields and plug them together to a multi-field simulation environment. This allows to substantially save excessive development time for such simulations and to exploit 'the best' available solution for each single field. In this context, a 'single field' can be a governing equation for a part of the overall domain, e.g., a flow equation in one part and an elastic structure equation in another part; or it can be a part of the right hand side of a partial differential equation, e.g., diffusion, advection or reaction; or it can be a set of equations for a subset of all physical fields, e.g., the momentum equations for velocities or the transport equations for a pollutant in a subsurface pollutant transport model; or it can be a specific scale model in a multi-scale approach based in scale separation; or it can even be a simulation component or a learning algorithm in a reinforcement learning setup. All these possible definitions of multi-field come with their own challenges. However, the 'plugging together' involves a lot of common technical and mathematical aspects that need efficient and robust solutions to make this idea work. In this presentation, I will give an overview of methods addressing (among others) the following questions:
How to distribute compute resources between different solvers? How to make several solvers exchange data efficiently? How to map data from one discretization to another? How to sustain / ensure stability in time dependent problems? How to do higher order time stepping? How to minimize communication overhead? How to handle physical fields with bounds?
At the end of the presentations, we show several application examples from classic fluid-structure coupling over biomechanics to subsurface flow and transport simulations realized with specialized single field solvers and our open source coupling library preCICE.

### A partitioned coupling approach for electromechanical simulations of skeletal muscles using preCICE

Homs-Pons, Carme (1); Villota-Narváez, Yesid (2); Doreti, Lalith Kumar (2); Klink, Marian (3); Lautenschlager, Robin (3); Göddeke, Dominik (3); Röhrle, Oliver (2); Schulte, Miriam (1)
*1: Institute of Parallel and Distributed Systems, Univeristy of Stuttgart, Germany*
*2: Institute for Modelling and Simulation of Biomechanical Systems, Univeristy of Stuttgart, Germany*
*3: Institute of Applied Analysis and Numerical Simulation, Univeristy of Stuttgart, Germany*

09:10

Macroscopic mechanical models of skeletal muscles often assume a uniform generation of active forces throughout the muscle. In contrast, electrophysiological models compute the muscle activation locally, and are able to capture spatial heterogeneity, but do not compute the muscle's deformation. Using a coupled electromechanical model allows us to simulate the macroscopic behaviour of the muscle while incorporating locally resolved activation dynamics.

We implement a coupled electromechanical model using OpenDiHu, an open-source high-performance simulation framework for neuromuscular simulations [1]. Our implementation follows the three-level muscle model proposed by Heidlauf and Röhrle [2]. Specifically, we couple a finite

element mechanical solver to an electrophysiological solver composed of an action-potential finite differences sub-solver, and a cellular PDE sub-solver.

Because the optimal timestep and spatial discretization is different for each solver, we need sub-cycling and mapping strategies to couple the solvers. Instead of using OpenDiHu's internal coupling tool, we couple the solvers using the coupling library preCICE [3]. By that we can access more complex mapping methods, and distribute the compute resources freely. In addition, using preCICE allows us to couple OpenDiHu solvers to external software. Since our recent work shows that OpenDiHu's mechanical solver is a bottleneck for performance [4], we investigate alternative mechanical solvers.

Overall, this work presents a partitioned coupling approach for simulating skeletal muscles by coupling OpenDiHu's electrophysiological solver to an external mechanics solver via preCICE. Thereby, OpenDiHu's electrophysiological solver can be used together with established biomechanics tools such as FEBio and LS-DYNA, making our coupled simulations more accessible and attractive to a broader user community.
References:

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**A staggered coupling framework for the optimization of multiphysics problems**

Kelemen, Máté; Warnakulasuriya, Suneth; Ansari, Talhah Shamshad Ali 09:30
*Technical University of Munich, Germany*

The staggered coupling of multiphysics problems has become an immensely successful method of tackling the complexities of strongly coupled phenomena, such as fluid-structure interaction [1]. At the same time, applications for high-fidelity optimization tasks with large numbers of design variables have also gained ground, especially methods using adjoint methods to compute the sensitivities of design variables. However, combining these categories of problems to form coupled optimization implies significant additional complexity for the coupling tool [2], such as computing cross-domain sensitivies, communicating and mapping sensitivities, or handling the control flow of adjoint solvers. A design to extend the existing interface of the CoSimulation coupling tool within KratosMultiphysics is presented, with a focus on

- modularity to support a wide range of single-domain solvers to couple,
- efficiency and scalability to make large coupled optimizations possible,
- and conciseness to minimalise extra work necessary to adapt existing solvers.

Additionally, standardized requirements are defined for single-domain solvers to compute cross-domain sensitivities. The proposed workflow is demonstrated through a few selected academic cases.

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**A Two-way coupled simulation framework for the prediction of fire-induced damage and smoke propagation in a building**

Palani, Arulnambi (1); Kandekar, Chaitanya (2); Weber, Wolfgang E. (2); Breuer, Michael (1) 09:50
*1: Chair of Fluid Mechanics, Helmut Schmidt University, Germany*
*2: Chair of Structural Analysis, Helmut Schmidt University, Germany*

Modeling of complex physical phenomena often requires the consideration of a multi-physics approach to describe the real-life situation. Such problems typically involve distinct physical domains governed by separate numerical models operating on different time and length scales, whose interactions necessitate the development of robust coupling strategies. Fire–structure simulation is a prime example, as it involves the strong coupling between fire dynamics and its structural response and vice versa. Fire events in buildings not only generate high temperatures and the spreading of smoke gases but also induce significant structural damages of the concrete structure. Such a kind of coupling is highly interdependent: The structural damage alters the flow of hot gases and smoke, while evolving fire conditions influence the thermal and mechanical stresses in the structure due to the temperature-dependent material behavior. Capturing these processes poses significant modeling and computational challenges and requires a two-way coupled computational framework that combines fire dynamics with structural analysis, enabling realistic predictions of both material degradation and fire propagation.

This contribution presents a fully coupled computational framework for the simulation of fire–structure interaction in buildings, with a particular focus on fire-induced damage in concrete structures. The dynamics of the fire, including the combustion, the convective, conductive and radiative heat transfer, and the complex turbulent fluid flow with smoke propagation, are
simulated using the widely used open-source software *Fire Dynamics Simulator* (`FDS`) [1]. `FDS` solves the filtered Navier-Stokes equations using a finite-difference method and employs the large-eddy simulation technique to model turbulent flows. The structural degradation of concrete, including damage, cracking, and thermo-mechanical spalling, is modeled using a phase-field approach implemented in a `FEniCS`-based solver. The capabilities of the phase-field fracture model is demonstrated using the Vulcain benchmark, providing a reference configuration for assessing its predictive capabilities under thermo-mechanical loading. The two solvers are bi-directionally coupled via the open-source coupling framework `preCICE` [2], enabling the exchange of a room's wall temperature data from the fire solver to the structural solver and the damage information from the structural to the fluid solver. More precisely, it means that the elevated temperature of the fire-exposed surface of the concrete wall considered determines the thermal input boundary conditions for the phase-field model. As damage evolves, the computational domain of the fluid flow simulation is dynamically updated to account for evolving cracks and damages in the concrete wall. The material degradation allows the leakage of smoke and hot gases into so far unaffected neighboring rooms, thereby influencing the progression of the fire throughout the building structure. The applicability of the proposed two-way coupled methodology implemented on a powerful HPC cluster is demonstrated through a representative real-world example involving a building with several rooms and considering the fire-induced thermal damage of a concrete wall and the resulting gas leakage.

**Time integration schemes for discrete electro-thermo-elastic systems based on GENERIC**

Reiff, Pit; Betsch, Peter; Franke, Marlon 10:10
*Karlsruhe Institut of Technology, Germany*

The consistent numerical treatment of the balance laws in multi-physical systems requires specialized time integration schemes. These integrators must preserve the invariants of the system,
as dictated by Noether's theorem, while adhering to the fundamental laws of thermodynamics:

conservation of linear and angular momentum, conservation of energy, and positive dissipation. The GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) is a two generator formalism which provides the foundation for constructing such integrators for (closed) discrete systems. As a first model problem, a thermo-visco-elastic pendulum under large deformations is considered. It incorporates heat exchange and viscous dissipation as challenging
features for the numerical integrators. Energy-Momentum-Entropy schemes, based on discrete gradients in the sense of Gonzalez [1], are developed for the model problem and their energy and entropy consistency is shown. The use of temperature, entropy, internal energy or total energy as independent variables is discussed. A focus is put on the special form of GENERIC according to Mielke [2] and the introduction of auxiliary variables like strain and its consequences on the structural properties of the discrete system. Extending the model problem to include electromagnetic forces enables a broader applicability to coupled electro-mechanical or magneto-mechanical systems, which are critical in modern engineering applications. The development of GENERIC-based integrators for discrete systems can be seen as a first step towards the development of GENERIC-based methods for continuum problems. The extension of GENERIC towards open systems as a tool for control is presented by extending the GENERICframework
in the spirit of port Hamiltonian (pH) systems. As a model problem, a simplified lumped parameter model of a microfluidic pump (see Franke et al. [3]) subjected to mechanical, thermal and electrical loads is discussed.

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## S07.02: Magnetic/piezoelectric materials

Date: March 17, 2026 16:30–18:30
Room: KII, M17.02
Chair(s): Kästner, Markus
Düster, Alexander

### Magnetic elastomers – coupling magnetic and mechanical interactions

Menzel, Andreas M. 16:30
*Otto-von-Guericke-Universität Magdeburg, Germany*

Notable mechanical impact results from external magnetic fields of moderate strength when magnetizable building blocks are combined with mechanically soft components. In basic realizations of such magnetizable composite systems, soft polymeric gels or elastomers serve as carrier “matrices” for particulate magnetizable inclusions. If these magnetizable inclusions are of a size starting from the upper colloidal scale, that is, micrometers, up to the submillimeter regime, pronounced reversible deformations can be achieved upon magnetization. Moreover, magnetization can serve to tune the elastic and dissipative properties in terms of rheological moduli of the overall system. Such materials are termed magnetosensitive or magnetorheological elastomers – here, in brief, magnetic elastomers.

On one hand, theoretical descriptions and numerical simulations of these materials are challenging. Both the induced magnetization fields and the mechanical deformation fields are spatially heterogeneous. On the scale of the inclusions, the magnetic fields need to satisfy boundary conditions at the surface of each individual inclusion, which distorts the fields. At the same time, rigid particulate inclusions lead to heterogeneous spatial distortions in the much softer elastic matrix. Consequently,

theoretical approaches need to introduce simplifying approximations to make progress. Alternatively, advanced computational approaches must be developed. On the other hand, the clear spatial separation between magnetizable and elastically deformable components makes the mathematical formulation of their coupling on the scale of the inclusions relatively straightforward and unambiguous. Induced mechanical distortions can be understood in a quite intuitive manner on that scale and may relatively conveniently be illustrated. From there, homogenization procedures can lead to more macroscopic material models and link to continuum descriptions.

As a logical step forward, we ask how the spatial arrangement of the magnetizable inclusions within magnetic elastomers affects their overall behavior. Besides the concern about optimized structural organization to obtain requested performance, we ask how to generate such textures in real systems, and how to theoretically describe and quantify corresponding processes of structural organization. Again, the behavior of the resulting structures must be linked to the overall behavior of the systems. This kind of approach requires concerted interactions between experimental and theoretical groups, while didactic concepts can serve to improve corresponding illustration and thus understanding. Such endeavors define present and future activities in the field.

Support of this research by the German Research Foundation DFG, specifically in the context of the Research Unit FOR 5599 on structured magnetic elastomers, is deeply appreciated.

**Constitutive modeling and finite element simulation of soft anisotropic magnetoactive elastomers**

Yazdandousthamedani, Alireza; Kanan, Anas; Kaliske, Michael 17:10
*Institute for Structural Analysis, Technische Universität Dresden, 01062 Dresden, Germany*

Magnetoactive elastomers (MAEs) are a class of smart materials composed of magnetic particles embedded in an elastomeric matrix. The mechanical response of MAEs can be tuned by applying an external magnetic field, allowing for adjustable stiffness and damping characteristics. Based on the magnetic properties of the particles, MAEs are classified as soft magnetoactive elastomers (s-MAEs) or hard magnetoactive elastomers (h-MAEs). s-MAEs contain magnetically soft particles such as carbonyl iron, which exhibit negligible hysteresis. When a magnetic field is applied and then removed, these materials are rapidly demagnetized. Conversely, h-MAEs, which consist of hard magnetic particles such as neodymium–iron–boron (NdFeB), display pronounced hysteresis and remanent magnetization, enabling the material to retain magnetic polarization after unloading.

Regarding magnetically soft inclusions, the spatial distribution of these particles influences the magneto-mechanical response of s-MAEs strongly. Depending on the curing conditions, these materials can exhibit isotropic or anisotropic microstructures. When cured under an external magnetic field, magnetic particles align in the direction of an applied magnetic field, forming chain-like structures, which lead to an anisotropic configuration of the composite. This alignment significantly enhances the field-induced mechanical response compared to isotropic s-MAEs. The anisotropic features of transversely isotropic s-MAEs make them particularly usable as adaptive devices, including vibration isolators, sensors, and tunable stiffness actuators.

Most of the related theoretical studies have focused on modeling the magneto-mechanical coupling of isotropic s-MAEs. Less research has been devoted to the modeling of the coupling behavior of anisotropic s-MAEs. To describe the nonlinear magneto-mechanical behavior in anisotropic structures consisting of a soft matrix and particle chains, two different frameworks are proposed in this contribution. The first approach employs an invariant-based formulation to describe the anisotropic coupling behavior of s-MAEs. The second formulation introduces a novel tensor-based model, which describes both the behavior of isotropic s-MAEs and the direction-dependent response of anisotropic s-MAEs. The new constitutive model is based on an additive decomposition of the total free energy into purely mechanical, magnetic, and coupled magneto-mechanical contributions. Both the magnetic and magneto-mechanical properties are assumed to depend nonlinearly on deformation. The proposed formulation is implemented into a finite element program, where its predictive capability under various magnetic and mechanical loading conditions is evaluated. The model successfully reproduces key features of the field-dependent mechanical response observed in anisotropic s-MAEs

and provides a robust theoretical basis, which can be used in the future for the design and optimization of MAE-based adaptive systems.

**A data-driven multiscale scheme for anisotropic finite strain magneto-elasticity**

Roth, Heinrich T.; Gebhart, Philipp; Kalina, Karl A.; Wallmersperger, Thomas; Kästner, Markus 17:30
*TU Dresden, Germany*

Structured magnetorheological elastomers (MREs) are composite materials exhibiting complex magneto-mechanical coupling effects, such as the magnetostrictive and magnetorheological effect. They consist of magnetizable particles arranged in chain-like structures within a soft elastomer matrix. As explicitly resolving their microstructure in real-world samples is infeasible, a multiscale modeling approach is necessary.
This work presents a framework for the macroscale modeling of structured MREs using physics-augmented neural networks (PANNs) [1,2,3], accounting for the material's anisotropic behavior. The proposed PANN macromodel satisfies key physical principles, including objectivity, material symmetry and thermodynamic consistency [1,2].
Assuming magnetostatic processes, the framework employs finite element (FE) simulations based on a variational principle for magneto-hyperelastic materials [4]. To address the quasi-incompressibility of the matrix, a four-field formulation is adopted.
The framework begins with data generation, where a representative volume element (RVE) undergoes sampled macroscopic magneto-mechanical loadings in FE simulations. The resulting homogenized microscale variables form a macroscale dataset for the training and testing of the PANN macromodel. The training follows a Sobolev approach and incorporates the automatic detection of the particle chain direction [3].
Once trained on the dataset, the PANN macroscale material model accurately predicts magnetization, mechanical stress, and total stress within the training data range.
Finally, the PANN model is used in a decoupled multiscale scheme as the material model of a macroscale FE simulation.
REFERENCES: [1] H.T. Roth et al., arXiv:2510.24197, 2025. [2] K.A. Kalina et al., CMAME 421, 2024. [3] K.A. Kalina et al., CMAME 437, 2025. [4] P. Gebhart, PhD thesis, TU Dresden, 2024.

**A multi-field FE analysis of Heusler alloys: computational materials under thermo-magneto-mechanical stimuli**

Alaeddini, Mobina; Schröder, Jörg; Vorwerk, Maximilian 17:50
*Universität Duisburg-Essen, Germany*

The current challenges posed by climate change create a need for new technologies based on advanced functional materials. Rising global temperatures increase the frequency and intensity of extreme weather conditions. These harsher climate patterns lead to a higher demand for cooling. As a result, energy consumption continues to grow, with air-conditioning (AC) systems making a major contribution. This rising demand for AC systems places strong pressure on existing energy resources. This situation highlights the need for more reliable and energy-efficient cooling technologies. Conventional vapor-compression systems cannot meet these needs without raising emissions further, which encourages the development of cooling alternatives. Novel AC systems are based on the so-called magnetocaloric effect. This effect describes the change in temperature in a magnetic material caused by external magnetic fields. Current research focuses on improving the mechanical and thermal properties of these materials, including Heusler alloys [2]. These alloys are strong candidates since their magnetic and structural responses can produce large temperature changes, making them attractive for solid-state cooling. To explore these effects in a controlled and quantitative manner, a detailed numerical analysis of the magnetocaloric behaviour using a variational phase-field formulation is conducted. The model follows a time-dependent Ginzburg-Landau equation and includes elastic, magnetic, and thermal energy effects. Within this framework, these contributions define the free-energy functional that governs the martensitic and austenitic phase transformation [2]. The magneto-mechanical coupling is described via the micromagnetic theory including linear elastic contributions [3]. Together, these components form a consistent multi-field framework for modeling

magnetocaloric materials. The study clarifies the interaction between magnetic and structural transformations in these alloys and supports the development of efficient magnetocaloric materials for sustainable cooling.

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**Modeling of losses in piezoceramics**

Sutter, Felix 18:10
*Physik Instrumente (PI) SE & Co. KG, Germany*

Loss phenomena in piezoceramics presents a major challenge in modern resonant and off-resonant driven actuator systems for high-precision positioning tasks. Hysteretic material behavior, which manifests as phase delay in deflection and current, requires complex control strategies in piezo-based systems. To achieve an increase in performance, various modeling approaches can be used to describe the loss characteristics of the material. A simple and popular approach for engineering applications is the use of complex material constants, which are representative of the phase delay. This frequency-domain approach, however, has the disadvantage that it is only valid for small dissipation rates and is also unsuitable for extended multiscale analyses. For a mechanism-based investigation of losses and the use of arbitrarily material models coupled to the microscale, a consideration in the time domain is necessary. The frequency-, temperature- and amplitude-dependent loss behavior of piezoceramics can thus be more accurately represented using sophisticated rate-dependent models - however, this requires a high computational effort in dynamic applications. One way to avoid these high computational costs is to use the harmonic balance method, which allows for the prediction of the complex, frequency-dependent loss behavior of piezoelectric components with moderate computational effort.

## S07.03: Magnetics/micromagnetics

Date: March 18, 2026 08:30–09:30
Room: KII, M17.02
Chair(s): Menzel, Andreas

**Cosserat micropolar flexomagnetism at finite strains**

Sky, Adam (1); Codony, David (2); Rudykh, Stephan (3); Zilian, Andreas (1); Bordas, Stéphane (1); Neff, Patrizio (4) 08:30
*1: Université du Luxembourg*
*2: Universitat Politècnica de Catalunya*
*3: University of Galway*
*4: Universität Duisburg-Essen*

We present geometrically nonlinear continuum models of flexomagnetism within the Cosserat micropolar framework and its reduced couple-stress theory. Magneto-mechanical coupling is introduced via a Lifshitz invariant linking the micro-dislocation tensor to the magnetisation vector. The models admit centrosymmetric materials with a single flexomagnetic constant and cubic-symmetric materials with two constants. We derive the governing equations from variational principles using scalar and vector magnetic potentials, and demonstrate the physical plausibility and computational feasibility through nano-beam simulations.

**Micromagnetic simulations based on the magnetic Gauss and Ampère's law**

Vorwerk, Maximilian; Schröder, Jörg 08:50
*University of Duisburg-Essen, Germany*

Magnetic materials in general, such as hard-magnetic neodymium-iron-boron (NdFeB) or soft-magnetic nickel-iron (NiFe), play a crucial role in driving power conversion devices as wind turbines, sensors, and electric motors [1]. Owing to their relevance for addressing technological and societal challenges, in particular the reduction of $CO_2$ emissions, these materials are being studied intensively. Current research targets improved performance, reduced dependence on critical raw materials, and a lower energy demand during manufacturing and processing. Numerical simulations, and in particular the finite element method (FEM), offer additional insights into the materials mechanisms itself to accelerate the development of these materials. Hence, reliable and robust simulation tools are in demand. Such reliable simulations of magnetic materials require some special care, in particular regarding the discretization of the magnetic field **H**. In this contribution, two different formulations based on a magnetic scalar potential and a magnetic vector, i.e., the magnetic Gauss law and Ampère's law, are considered to represent the magnetic field. To ensure the uniqueness of the magnetic vector potential, the Coulomb gauge condition is imposed [2]. This work demonstrates the workability of both formulations, applied to a FEM based micromagnetic framework, in terms of suitable numerical examples and highlights the individual advantages.

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**A micromagnetic simulation of zigzag domain wall formation**

Yılmaz, Çağlar; Vorwerk, Maximilian; Schröder, Jörg 09:10
*University of Duisburg Essen, Germany*

Understanding the magnetic domain configurations in magnetic materials is crucial for explaining magnetization processes and the properties of ferromagnets [1]. Investigations of domain structures reveal how various interactions, such as magnetostatic, exchange, and anisotropy effects, work together to stabilize the ferromagnetic domain state. The magnetic properties of a thin film are strongly influenced by its domain configuration; therefore, achieving precise control over a film's magnetic response requires detailed knowledge of its micromagnetic structure. Insights into the arrangement of domain patterns are essential for many technological applications, including spintronic devices. One commonly observed type of domain wall structure is the charged domain wall. These walls typically take on a zigzag shape and form between regions where the magnetization directions point directly toward each other. This zigzag geometry is understood to lower the magnetostatic energy by spreading out the magnetic charge, which reduces the local charge density at the cost of increasing the overall wall length, with the charge distributed along both sides of the wall [2]. A quantitative understanding of this energy balance and the resulting domain-wall configurations requires a theoretical framework capable of resolving magnetization at the microscopic scale. The theory of micromagnetism [3–5], a continuum theory, describes the behaviour and arrangement of magnetic moments and therefore provides a suitable tool for analyzing magnetic properties and optimizing experimental processes. In this context, we performed finite element simulations to investigate the formation of zigzag domain walls in magnetic thin films under different conditions. We examined the influence of film thickness, edge geometry, and the presence of precipitates on domain-wall formation.

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## S07.04: Coupled flow problems

Date: March 18, 2026 14:00–16:00
Room: KII, M17.02
Chair(s): Radtke, Lars

### Modeling and Numerical Simulations of Space-Time Non-Newtonian Fluids with Internal Variables

Choi, Yongbin; Soleimani, Meisam; Wick, Thomas; Junker, Philipp 14:00
*Leibniz University Hannover, Germany*

This talk is on a space-time model for non-Newtonian fluid flow based on Hamilton's principle, incorporating an internal variable to account for spatial and temporal variations in the viscosity. The internal variable evolves in response to local flow conditions, enabling a more refined and dynamic modeling of complex non-Newtonian behaviors. Two models, referred to as Type 1 and Type 2, are formulated based on different free energy fluid potentials. The Type 1 model captures the viscosity evolution through the interaction between velocity and displacement gradients, whereas the Type 2 model is driven by the strain magnitude. Both models are capable of reproducing shear-thinning and shear-thickening behaviors within a unified and thermodynamically consistent framework. In extension to
conventional models defined as non-linear algebraic relations between stress and velocity gradient, the proposed framework naturally incorporates viscosity evolutions in both space and time. The numerical formulation is based on a space-time finite element method, where velocity, displacement, and pressure fields are globally discretized, while the internal variable is computed locally at each integration point. Simulation results for channel and cylinder flow problems demonstrate that the proposed models effectively capture a wide range of non-Newtonian flow characteristics.

### Modeling of actively forced close-contact melting in latent heat storage systems for performance evaluation

Bünning, Jonas; Bhattacharya, Dipankul; Kowalski, Julia 14:20
*RWTH Aachen, Germany*

Latent heat storage systems constitute a promising technology for thermal energy storage applications. They function by absorbing or releasing large amounts of energy as the material phase changes. A critical metric for these thermal storage systems is the time it takes to charge and discharge heat. For latent heat storage systems based on a liquid-solid phase change material (PCM), it has been shown that charging speed can be increased by actively forcing the solid PCM against a heat source. The latter induces a process referred to as close-contact melting, in which phase-change occurs in a microscale contact film. Coupled close-contact melting models are sought to predict the performance of the latent heat storage systems in terms of charging speed. One of the big challenges for such models is the fact that charging speed is determined by thermo-fluidmechanically coupled processes in the contact film.
In this work, we present two methods for computing the charging speed of such a force-enhanced thermal storage system. The first method is based on an analytical model and is inspired by existing

contact melting solutions. The second method comprises a fully resolved coupled numerical model that accounts for fluid flow governed by the Navier-Stokes equations within the liquid PCM, as well as melting and refreezing according to a physically consistent interface condition referred to as the Stefan condition. The results of both the analytical and numerical model are compared to experimental data obtained from literature. For both models, we find a good agreement to experimental results. We also show that the presented models offer better agreement with experimental results than existing analytical models. In general, we find that for values within the practical limits of latent heat storage systems, its behavior can be largely characterized by the Stefan number alone.

**Coupled Multi-X Modeling in Sea Ice Dynamics**

Pathak, Raghav (1,2); Seyedpour, Seyed Morteza (1,2); Kutschan, Bernd (3); Thoms, Silke (3); Ricken, Tim (1,2)

*1: Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Germany*

*2: Porous Media Lab, Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Germany*

*3: Ecological Chemistry, Alfred Wegener Institute, Germany*

14:40

Sea ice plays a pivotal role in the climate dynamics of polar regions by mediating the interactions between the atmosphere, ocean, and ecosystem. Its complex microstructure, a porous matrix of solid ice, liquid brine, and dissolved salts, not only governs its thermophysical properties but also hosts critical biogeochemical processes. This presentation introduces a comprehensive "Multi-X" numerical modeling framework designed to simulate sea ice formation and its associated biogeochemical dynamics through an integrated multi-phase, multi-component, multiscale, and multiphysical approach. The physical foundation of the model is the Extended Theory of Porous Media (eTPM), which provides a thermodynamically consistent description of sea ice as a biphasic medium. At the microscale, a phase-field model based on the Landau-Ginzburg approach is employed to resolve dendritic ice crystal growth and the formation of brine channels, capturing the coupled evolution of salinity and pore geometry under varying environmental conditions. These microscale equilibrium solutions are then upscaled to the macroscale eTPM framework via an offline coupling strategy, enhancing the model's accuracy by incorporating pore-scale-dependent properties. This physical model is further extended by coupling it with a biogeochemical (BGC) module, described by a system of ordinary differential equations, to simulate photosynthetic dynamics, nutrient uptake, and carbon assimilation within the brine network. This coupling allows for the simulation of seasonal biological activity and its dependence on the evolving microstructure of the sea ice. To address the computational expense of these high-fidelity simulations, a surrogate model based on Principal Component Analysis (PCA) and Singular Value Decomposition (SVD) is introduced. This reduced-order model efficiently approximates BGC outputs, enabling rapid assessment of biogeochemical responses under various scenarios. The presented Multi-X framework provides a detailed and extensible modeling pipeline for investigating sea ice dynamics and their profound implications for polar biogeochemistry and global climate processes.

**Towards modelling of the friction coefficient in wet grinding processes**

Thunich, Paul; Müller, Michael

*TU Braunschweig, Germany*

15:00

In grinding processes, process parameters are currently set based on experience or empirical trial-and-error tests since little knowledge about basic interactions between process parameters exists, and contrary influences must be balanced. Especially when developing new cutting fluids, a conflict between cooling effects and hydrodynamic load-bearing effects arises. To resolve this conflict, a model is developed to investigate these interactions and to optimise wet grinding processes.

The model can be divided into two parts. On a macroscopic level, the Reynolds equation is used to model the hydrodynamic pressure build-up, while a newly developed cavitation algorithm based on the shifted penalty method is utilised. Additionally, the influence of the grinding wheel's porous structure on the pressure distribution is examined by coupling the consideration of the porous domain to the Reynolds equation. Numerical analysis at this scale is conducted via isogeometric analysis (IGA)

based on NURBS. This approach efficiently computes hydrodynamic parameters and enables coupling with a thermal consideration of the fluid while maintaining a reasonable system size for a monolithic approach.

The second part of the process modelling is the consideration of the engagement of the grinding grains. To account for the contact forces of the cutting mechanism, a microscopic model has been built based on a probability density function derived from measured deterministic height profiles. This approach, adapted from metal forming simulations, enables a comparably fast computation of the real contact area and an approximate penetration depth of the abrasive grains into the workpiece. By accounting for the influence of surface roughness and contact areas on the hydrodynamic pressure build-up at a microscopic scale, this model opens up the possibility of approximating a global coefficient of friction by linking from the microscopic scale back to the macroscopic scale.

This integrated modelling framework demonstrates how considerations of different sub-processes can be combined to create a lean modelling procedure for optimising wet grinding processes through numerical analysis.

**Simulation and validation of an solvent-based CO2 capture process**

Verma, Rakhi (1); Mirlekar, Gaurav (2); Mauss, Fabian (1); Øi, Lars Erik (3)

*1: Chair of Thermodynamic/Thermal Process Engineering, Brandenburg University of Technology Cottbus-Senftenberg, 03046 Cottbus, Germany*
*2: Department of Electrical Engineering, Information Technology and Cybernetics, University of South-Eastern Norway, 3918 Porsgrunn, Norway*
*3: Department of Process, Energy and Environmental Technology, University of South-Eastern Norway, 3918 Porsgrunn, Norway*

15:20

Global greenhouse gas (GHG) emissions must peak immediately and decline toward net-zero by 2050 to meet the Paris Agreement targets. Since fossil fuel based thermal power plants continue to dominate global electricity production, integrating these systems with Carbon Capture and Storage (CCS) technologies is essential for mitigating $CO_2$ emissions during the energy transition. Post-combustion $CO_2$ capture (PCC) using chemical absorption is one of the most mature CCS options. Under variable renewable energy conditions, PCC systems must maintain stable $CO_2$ removal performance despite fluctuations in flue-gas flow and temperature. Accurate process modelling both steady-state and dynamic is therefore crucial for designing and controlling CCS processes under realistic, flexible operating conditions.

This work develops and validates a first-principles, model-based simulation of the $CO_2$ absorption–desorption test rig at the University of South-Eastern Norway (USN). The rig, operated since 2010, uses 30 wt% monoethanolamine (MEA) and provides high-quality experimental data across a wide range of conditions, including variations in gas and liquid flow rates, temperatures, and $CO_2$ concentrations. These data serve as a benchmark for evaluating the predictive capability of process simulation tools used in CCS research.

We first perform the steady-state simulations to establish the baseline accuracy of the simulation model. The model is fitted to experimental data for CO2 capture removal efficiency as a function of varying gas flow, liquid flow, temperature and CO2 concentration in inlet gas. Steady-state validation is essential for confirming that the implemented thermodynamic models, mass-transfer descriptions, and equipment parameters accurately reflect the physical system. Once the model performance is verified at steady conditions, the investigation is planned to extend to the dynamic simulations. Dynamic modelling allows assessment of the system's transient response to operational disturbances, which is vital for flexible operation and for the development of optimal control strategies.

The simulation results will be systematically compared with experimental measurements of $CO_2$ removal efficiency and energy performance from the USN rig. Through this comparison, the study aims to evaluate the suitability of process simulator (e.g., Aspen HYSYS) for representing MEA-based PCC under various operating conditions.

The validated model will support future work on advanced control frameworks for PCC systems, ultimately contributing to improved operational flexibility and reduced $CO_2$ emissions in CCS-integrated thermal power production.

**Modeling of constrained thin films in hydrogen environment**

Gisy, Johannes (1); Seiler, Magdalena (2); Wagner, Stefan (2); Pundt, Astrid (2); Böhlke, Thomas (1)

*1: Institute of Engineering Mechanics, Chair of Continuum Mechanics, Karlsruhe Institute of Technology (KIT), Germany*

*2: Institute for Applied Materials, Material Science and Engineering, Karlsruhe Institute of Technology (KIT), Germany*

15:40

Thin metal films are exposed to hydrogen (H) such that hydride formation and phase stability can be investigated. The hydride-forming metal, i.e. palladium (Pd) or niobium (NB), is sputtered on a substrate material, i.e. sapphire which is inert to H exposure. The substrate material's thickness is several magnitudes larger than that of the metal film. Due to the H-induced lattice expansion of the adhered film, the composite structure will bend and stresses arise, accordingly. Depending on the stress state and the temperature, hydride formation is possible, or suppressed [2]. However, inelastic deformations affect the phase stability such that the hydride stability is altered for a fixed temperature. Experimental studies in Colla et al. [1] investigate the creep behavior of thin Pd films, revealing a rate dependency of the plastic flow. Thus, it becomes relevant in which time period the specimen will be loaded and/or unloaded with specified amount of H.

To support these investigations, a Finite-Element (FE) model to account for the composite structure that is able to bend, is necessary. A (thermo-)chemo-mechanical model including a rate dependent plastic potential is introduced for the thin film accounting for H diffusion and inelastic deformation. The focus is on the chemo-mechanical coupling. In a first attempt, state-of-the-art approaches are considered to see where additional modeling needs to be done. The thin film is placed on a reference substrate resembling a metal-ceramic bimetal strip. Due to the high difference in thickness, the material model of the substrate has to be modified by defining an equivalent stiffness, to reduce the thickness of the substrate. Thus, the material model of the substrate has to be modified. The chemical model includes full coupling between the diffusion flux and the mechanical pressure [3]. Therefore, the chemical potential depends on the mechanical pressure as well which needs to be taken into account when the phase stability is investigated. Preliminary results regarding the FE model as well as the material model of the thin film will be presented.

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**S07.05: Phase-field models**

Date: March 18, 2026 16:30–18:30
Room: KII, M17.52
Chair(s): Aldakheel, Fadi

**Continuum-Thermodynamic Formulation of Phase-Field Models Using Internal State Variables**

Prahs, Andreas (1); Schneider, Daniel (1,2); Nestler, Britta (1,2) 16:30
*1: Karlsruhe Institute of Technology (KIT)*
*2: Karlsruhe University of Applied Sciences*

Phase-field models provide an efficient framework for the description of interface motion and microstructure evolution in solids [1]. In classical formulations, the phase-field variable is typically introduced as an additional degree of freedom, and its governing equation is derived from variational principles or the principle of virtual power, with the diffuse nature of interfaces assumed from the outset.

In the present contribution, we adopt an alternative perspective and interpret the phase-field order parameter as an internal state variable within continuum thermodynamics, following the conceptual arguments in [2]. Moreover, the phase-field method is regarded as an approximation of sharp-interface theory for continua with singular surfaces [3]. Based on the Clausius–Duhem inequality, the evolution equation of the order parameter is derived in a thermodynamically consistent manner [4]. The resulting framework naturally incorporates heat conduction, thermomechanical coupling, and energetic contributions associated with phase transformations, including latent heat, within the diffuse interface region. Finally, the obtained evolution equation is discussed in relation to classical variational phase-field formulations. The proposed approach provides a consistent thermodynamic foundation for phase-field modeling.

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**A Thermomechanically Coupled Model including Latent Heat based on a Multiphase-Field Approach**

Hu, Binzi (1); Prahs, Andreas (1); Reder, Martin (2,3); Schneider, Daniel (2); Nestler, Britta (1,2,3) 16:50
*1: Karlsruhe Institute of Technology (KIT), Institute of Nanotechnology (INT-MSS)*
*2: Karlsruhe Institute of Technology (KIT), Institute for Applied Materials (IAM-MMS)*
*3: Karlsruhe University of Applied Sciences (HKA), Institute of Digital Materials Science (IDM)*

In the domain of material science, computational simulations of microstructure evolution offer a resource-efficient option for the design and optimization of materials. In order to provide a quantitative description of microstructure evolution, it is essential to capture all relevant physical effects in the underlying numerical models. The multiphase-field method (MPFM) has become an established approach for modeling and simulating microstructures involving multiple phases [1]. The MPFM enables the efficient computation of the domains occupied by evolving phases and the corresponding moving interfaces in-between. It is widely used for applications such as grain growth and solidification. In phase transformation processes involving plastification, such as martensitic phase transformations, the thermomechanical coupling is often neglected. Nevertheless, for non-vanishing thermal expansion coefficients, taking into account coupling terms and latent heat can affect the evolution of the temperature field, even at small strains and strain rates. The plastic stress power and thermomechanical coupling terms are both considered to act as heat sources or sinks [2]. Moreover, the release of latent heat plays an important role in numerous phase transformation processes, necessitating its consideration to ensure the accuracy of the predicted microstructure evolution. The presented contribution focuses on the role of latent heat in the context of displacive phase transformations [3]. To this end, the evolution of an elastoplastic inclusion embedded in an elastoplastic matrix is analyzed under various loading conditions.

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**Multi-Dimensional Phase-Field Modeling of Chromium Oxidation with Realistic Thermodynamic and Kinetic Parameters**

Löps, Paul (1); Roth, Stephan (1); Schlereth, Clara (2); Donchev, Alexander (2); Galetz, Mathias (2); Kiefer, Bjoern (1)
*1: Institute of Mechanics and Fluid Dynamics,TU Bergakademie Freiberg, Germany*
*2: DECHEMA-Forschungsinstitut, Germany*

17:10

High-temperature oxidation of chromium-containing steels is controlled by complex interactions of diffusion, reaction, and phase transformation processes that produce protective $Cr_2O_3$ layers. While one-dimensional studies have demonstrated agreement with laboratory measurements, real components exhibit strong spatial inhomogeneities—particularly at corners, edges, and surface curvature—requiring a fully multi-dimensional treatment.
In this contribution, we extend the multi-phase, multi-component model based on mixture-theoretical mass conservation and chemical-potential-driven diffusion discussed in [1, 2]. As a specific application example of the general framework, we consider the case of five chemical components and two phases and track diffuse phase interfaces through Allen–Cahn and Cahn–Hilliard equations. The approach accounts for density changes associated with chromium oxidation following reaction formulations, cf. [3]. Here, we apply unscaled, experimentally validated material parameters to enable two-dimensional simulations under realistic operating environments relevant to high-temperature applications in the chemical industry as well as the energy sector, e.g., electrolysis for hydrogen production.
The finite element implementation was done in Abaqus using the user element interface (UEL) as well as the in-house element library UELLib. Applying the routine in a spatial problem allows us to capture oxide growth, chromium depletion, and interface migration on complex geometries. The simulations reveal pronounced spatial variations—outer corners are chromium-starved and develop thinner protective layers, while inner corners exhibit enhanced diffusion pathways and accelerated oxide growth. Using the experimentally measured diffusion parameters done by DFI as well as the chemical potentials based on CALPHAD methods allows for quantitative predictions of local layer thicknesses and oxidation rates. This enables direct comparison with spatially resolved laboratory measurements from one-dimensional experiments.
The results demonstrate that the physically calibrated model based on the one-dimensional experiments captures not only the global oxidation behavior but also the critical geometric sensitivities that govern component lifetime in multi-dimensional applications. This provides a rigorous foundation for predictive design and optimization of corrosion-resistant components in high-temperature technologies.

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**Continuous modeling of the anodic material dissolution in electrochemical machining using a phase field approach**

Schmidt, Annika; Waimann, Johanna
*Ruhr University Bochum, Germany*

17:30

The electrochemical machining (ECM) process is a non-conventional machining process which allows the contactless machining of arbitrarily shaped workpieces through anodic material dissolution. As

there is no direct contact between the tool and the workpiece, high surface finishes can be achieved without causing heat affected rim zones or inducing residual stresses in the material [1]. However, identifying the required process parameters necessitates multiple time- and cost-intensive test runs in the laboratory. By developing precise material models which realistically estimate the machining results of the ECM process, the desired process parameters could be determined in advance, saving resources and costs.

Over the years, different numerical models were established, whereby most of them require a remeshing procedure of the anodic surface at every time step. In order to avoid remeshing, van der Velden et al. [2] introduced a continuous modeling approach, where the electrical boundary value problem is solved using homogenized material parameters. In their work, the material dissolution is governed by an evolution equation which considers an activation function to ensure contact between the metal and the electrolyte in the dissolution zone. However, this activation function leads to an undesired mesh dependent anodic material dissolution. To overcome this, we present a new model, based on a phase field formulation [3], which, in this work, is derived in a variational manner, assuming quasi-stationary conditions. Here, the dissolution variable serves as the scalar phase field quantity and its evolution in time is governed by the Allen-Cahn equation. To validate the derived phase field approach, the influence of the applied electric current and the interface kinetics parameter on the anodic material dissolution is investigated. Furthermore, we consider the effects of different initial surface roughnesses of the workpiece as well as of different tool shapes.

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**Coupled phase-field-mechanical modeling of solid-state sintering**

Ivannikov, Vladimir (1); Munch, Peter (2); Cyron, Christian (1,3)

*1: Helmlholtz-Zentrum Hereon, Germany*
*2: Technical University of Berlin, Germany*
*3: Technical University of Hamburg, Germany*

17:50

Solid-state sintering is a materials processing technique in which a compact of powder particles is heated to a temperature below its melting point, causing the particles to bond and densify through diffusion-driven mass transport. This process leads to neck growth between particles, reduction of porosity, and overall densification without the formation of a liquid phase.

At the microscopic level, solid-state sintering is governed by atomic diffusion along surfaces, grain boundaries, and through the bulk. Among these three diffusion paths, the grain boundary diffusion has an important side effect. The outflow of atoms from the neck centers to their surfaces results in appearance of compressive local stresses, which turn out to be the driving force for shrinkage during sintering.

One of the numerical methods widely used for modeling microstructural evolution in materials science is the phase-field method. In the context of sintering processes, the governing equations typically consist of the Cahn–Hilliard and Allen–Cahn equations. While they capture mass transport phenomenon, they completely omit the mechanical part of the process underlying the shrinkage effect. To account for the latter, the rigid-body motions of particles driven by the so-called sintering forces was introduced in the seminal work of Wang. These forces are, however, directly converted into advection velocities for the phase fields, bypassing a consistent mechanical description of deformation. As a result, the model violates fundamental continuum mechanics principles and exhibits non-physical

behavior, such as a spurious dependence of the shrinkage rate on the number of particles in the system.

In the present contribution, we address these shortcomings by formulating a volumetrically coupled phase-field-mechanical model for sintering. The phase-field evolution equations are fully coupled to the linear-elastic balance of momentum, where the sintering forces enter naturally as distributed body loads. This multi-field formulation yields mechanically consistent advection velocities for the phase fields and introduces long-range particle interactions through the elastic field, thereby restoring physically meaningful shrinkage behavior.

From a numerical perspective, the resulting coupled problem is solved using a monolithic multi-field approach combined with implicit time integration. The implementation is based on the hpsint framework, a high performance matrix-free finite element solver tailored to large-scale multi-particle sintering simulations, featuring efficient block preconditioning strategies and advanced grain-tracking capabilities. The code employs deal.II and Trilinos libraries.

We first study a simple academic configuration consisting of a one-dimensional chain of identical particles to systematically analyze the deficiencies of the original Wang model and to demonstrate how the proposed coupled formulation resolves them. We then present a set of two- and three-dimensional benchmark problems to illustrate the robustness, physical consistency, and numerical advantages of the proposed coupled phase-field-mechanical approach.

**A phase-field model for the evolution of shape and chemical composition of volcanic olivine crystals**

Haddenhorst, Hendrik Holger; Waimann, Johanna; Chakraborty, Sumit; Hackl, Klaus 18:10
*Ruhr University Bochum, Germany*

Olivine crystals are present in the magmatic environments of volcanoes. Various methods, for example Diffusion chronometry, are used to access the diffusion record of these crystals and understand the movement in a magmatic environment prior to an eruption [1]. However, recrystallization is a limiting factor which prevents access to a crystal's diffusion history. The qualitative effects from the coupling of mechanical and chemical processes have been demonstrated in both experimental settings [2] and field observations [3], whilst a quantitative description has not been achieved yet.

In this presentation, we introduce a phase-field model, which couples the evolution of the concentration of diffusing elements with lattice strain and the resulting increase of the dislocation density, as well as the evolution of the size and shape of the crystal. This approach is based on a model for an idealized spherical crystal [4], the phase-field method enables us to consider arbitrary initial shapes. Furthermore, thanks to its general nature, the model can be adapted to be used for other types of crystals or even other applications which are not related to the field of geology.

We present the introduction of the model with results and discuss possible pathways to consider anisotropy.

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## S07.05.02: Porous media

Date: March 18, 2026 16:30–18:30
Room: KII, M17.02
Chair(s): Markert, Bernd

### Variational formulations for the dynamics of fluid-saturated porous media

Khurshid, Hamza; Polukhov, Elten; Keip, Marc-Andre 16:30
*University of Stuttgart, Germany*

Porous materials are widely encountered in engineering applications where their dynamic response plays a critical role. Study of such behavior is of utmost importance in many problems to understand the associated acoustics, impact, and vibration phenomenon in these materials. Examples can be seismic wave propagation in soils and ultrasound wave propagation in biological tissues. Accurate modeling of these phenomena requires accounting for solid and fluid inertia, acceleration effects, and transient fluid-solid interactions.

The dynamic behavior of fluid-saturated porous media has been studied extensively since the seminal work of Biot, who developed a theoretical framework for elastic wave propagation in porous materials across low- and high-frequency regimes [1,2]. Based on this foundation, further variational formulations and finite-element implementations have been proposed for poroelasticity [3,4]. In this contribution, we extend the variational two-field formulation of Miehe et al. [5] to describe the dynamic response of porous materials within the small-strain regime. The proposed time-discrete family of variational formulations employs displacement and fluid-flux fields as primary variables. Fluid flow is modeled using Darcy and Darcy–Forchheimer-type laws, while Rayleigh-type damping is incorporated to represent dissipation in the solid skeleton and to enhance the stability of the time integration scheme. The formulations are implemented using the standard finite-element method, and numerical examples are presented to illustrate the dynamic response and wave propagation characteristics of the proposed model.

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**Existence and Numerical Methods for Coupled Degenerate Darcy Flow**

Ray, Nadja (1); Duran, Omar (2); Schulz, Raphael (1); Kumar, Kundan (3) 16:50

*1: KU Eichstätt-Ingolstadt, Germany*
*2: Stanford University, USA*
*3: University of Bergen, Norway*

Alterations in hydrodynamic parameters such as porosity and permeability are key determinants of fluid flow in porous media. Physical, chemical, or biological processes may lead to pore-space clogging, resulting in the degeneracy of these parameters. We study a coupled degenerate Darcy–Darcy model in which degeneracies may arise in either of the coupled subdomains. Building on the framework of transformed unknowns and weighted function spaces introduced by Arbogast [1], we establish existence and uniqueness of solutions, as well as a priori error estimates for the corresponding discretized problem. Numerical experiments are presented to evaluate the convergence behavior and to compare formulations based on transformed and non-transformed unknowns.

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**Performance of a mixed least-squares finite element formulation with application in poroelasticity**

Hegde, Manu; Schwarz, Alexander; Bluhm, Joachim; Schröder, Jörg 17:10

*University of Duisburg-Essen, Germany*

A mixed least-squares finite element method (LSFEM), previously proposed in [1] for the analysis of the geometrically nonlinear theory of porous media (TPM), is further investigated in this work. Finite deformation of a fully saturated, incompressible solid–fluid binary system is studied using the LSFEM. The stress and deformation of the solid phase, along with the pore pressure and velocity of the liquid phase, constitute four independent fields in this formulation. The normal-flux preserving, vector valued Raviart–Thomas (RT) functions are employed to discretize the stress and velocity fields, while the displacement and pressure fields are approximated using conventional Lagrange polynomials (P). The LSFEM avoids the intricacies associated with satisfying the inf–sup (or LBB) condition required in mixed Galerkin finite element methods [2] to ensure stability. Another key advantage of the LSFEM is that non-self-adjoint differential operators also result in symmetric positive-definite system of matrices. The error minimization approach adapted in LSFEM makes the role of residual weights crucial in deciding the convergence characteristics. Therefore, in this study, the performance of higher order RT-P elements is evaluated against the canonical consolidation problem. A parametric study is carried out to describe the effect of respective weights on the convergence of analysis. The behavior of each residual with the usage of different combination of RT and P functions is also brought into context. The suitability of the developed LSFEM for the simulation of fluid saturated porous media with incompressible constituents is thus demonstrated.

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**Steady vibration problems in the coupled theory of Moore-Gibson-Thompson thermoporoelasticity**

Svanadze, Merab 17:30
*Ilia State University, Georgia*

In this talk, a linear coupled model of Moore–Gibson–Thompson thermoporoelasticity is proposed. The basic 3D boundary value problems (BVPs) of steady vibrations are thoroughly investigated using the potential method (the boundary integral equation method). The governing equations for motion and steady vibrations within this model are presented. The coupled system of equations is formulated in terms of the displacement vector field and the changes of the following three mechanical values: the volume fraction of pores, the fluid pressure in pore network, and the temperature of a porous material. The uniqueness theorems for classical solutions of both internal and external BVPs are proved. Surface and volume potentials are introduced, and their essential properties are established. Singular integral operators relevant to the BVPs are defined, and their symbolic determinants and indices are calculated. Finally, the existence theorems for classical solutions to these BVPs are proven using the potential method and the theory of 2D singular integral equations.

**Acknowledgements:** This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [Grant # FR-23-4905].

**The influence of liquid-gas mixture compressibility on Natural Hydraulic Fracturing processes**

Rivas, Yann; Ehlers, Wolfgang; Wagner, Arndt 17:50
*University of Stuttgart, Germany*

Natural hydraulic fracturing (NHF) describes a fracture event in saturated subsurface rock formations caused
by changes in local pore pressures due to rapidly changing boundary conditions, cf., e. g., French et al. [3], Boutt et al. [1] and Wang et al. [5]. The present high pore pressure gradients in low-permeable rocks therefore result in high tensile stresses in the solid rock material and subsequently cause fracturing. NHF stays in contrast to the broadly studied hydraulic fracturing, where a pressurised liquid is forced into a rock formation to artificially create a fracture network. In Wang et al. [5], a recent approach to describe NHF is presented based on Ehlers & Luo [2], which uses a Theory of Porous Media (TPM) phase-field approach describing a porous solid which is fully saturated with an incompressible liquid in combination with experiments. In this talk the focus lies on the extension of this existing TPM-phase-field model by considering a compressible liquid-gas mixture as the pore content of the porous medium. Studying the effect of a compressible liquid-gas mixture in NHF is motivated by the observed influence of the gas phase in hydraulic fracturing problems studied in Sonntag et al. [4]. Therein, it was shown that the compression of the gas phase slows down the fracture propagation. However, for the scenario of natural hydraulic fractures, where the liquid-gas mixture likely expands under pressure relaxation, the opposite phenomenon is expected. This could be of devastating relevance near or at CO2 injection sites during man made or natural geological events.

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**A porous media approach for multiphysics modeling of proton exchange membrane water electrolysis components**

Antonini, Alberto (1); Xotta, Giovanna (2); Salomoni, Valentina (2); Aldakheel, Fadi (1) 18:10
*1: Leibniz University Hannover, Institute of Mechanics and Computational Mechanics, IBNM*
*2: University of Padua, Department of Civil Environmental and Architectural Engineering, DICEA*

The climate crisis is one of the most critical challenges of the modern era, making a rapid reduction of greenhouse gas emissions essential. In this context, renewable energy technologies and green hydrogen storage play a central role in enabling a carbon-neutral energy system. Proton Exchange Membrane Water Electrolysis (PEMWE) is a key technology for high-purity hydrogen production, due to its high efficiency, fast response to fluctuating power inputs, and capability to operate at high current densities and pressures.

This work presents a unified multiphysics modeling framework for PEMWE systems, focusing on the Nafion membrane (PEM) and the cathode Gas Diffusion Layer (GDL). Nafion, the most widely used solid electrolyte for water electrolysis, is a perfluorosulfonic acid polymer characterized by a nanostructured porous morphology formed by water-filled ionic channels embedded in a polymeric matrix. Water uptake enables proton transport through the aqueous phase, while fixed anionic groups bound to the polymer backbone govern the membrane's electrochemical and mechanical behavior.The framework is formulated within the Theory of Porous Media (TPM), extended through the Theory of Mixtures (TM) to account for dissolved species and mobile ions in an electrodynamic setting [1]. This approach allows a consistent description of the strong coupling between membrane deformation, water transport and pressure within nanopores, and proton migration driven by concentration and electric potential gradients [2].

The cathode GDL is modeled as a deformable porous medium that plays a key role in gas transport, water management, and electrical conduction. Although carbon-based GDLs can be employed at the cathode due to the less aggressive electrochemical environment compared to anode, they exhibit a pronounced sensitivity to mechanical compression. Assembly-induced clamping pressures generate localized stresses that may partially collapse the porous structure, leading to permanent deformation, reduced porosity and permeability, and degraded mass transport. Accurate constitutive modeling of cathode GDLs is therefore essential. Carbon-based GDLs exhibit foam-like mechanical behavior, with pressure-dependent yielding and sensitivity to the stress state. To capture these features, a plasticity formulation, originally developed for granular materials, is adopted using a non-associative plasticity model which provides a flexible and robust description of the inelastic response of porous and compressible media, including pressure sensitivity, dilatancy, hardening, and large deformations, making it suitable for modeling the mechanical behavior of cathode GDLs.

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**S07.06: Porous media & metamaterials**
Date: March 19, 2026 08:30–10:30
Room: KII, M17.02
Chair(s): Jänicke, Ralf

**Modelling Material Injection Into Porous Structures With the Theory of Porous Media: (In-)Consistency Under Local Thermal Non-equilibrium Conditions**

Völter, Jan-Sören Lennart; Ricken, Tim; Röhrle, Oliver 08:30
*University of Stuttgart, Germany*

Percutaneous vertebroplasty is a medical procedure in which bone cement is injected into a mechanically unstable vertebral body. The vertebral body is a porous bone structure, fully saturated with red bone marrow. The bone cement (fluid) displaces the bone marrow (fluid) and penetrates the unstable bone structure (solid). After this injection, the bone cement turns solid and stabilises the bone structure. This is the biomechanical application we consider, model and simulate.

Our application poses a non-isothermal problem, in which one solid constituent and two fluid constituents interact. Our application is non-isothermal since bone cement starts at room temperature, whereas the vertebral body starts at body temperature. This even warrants the consideration of local thermal non-equilibrium (LTNE) conditions, wherein the heat transfer between the constituents is to be modelled and simulated.

In a previous contribution, we presented a thermo-mechanical, multi-phase, continuum model describing such material injection processes into porous media. We derived our model using the Theory of Porous Media (TPM), wherein we rigorously applied the underlying, thermodynamic principles of constitutive modelling. In conclusion, due to the assumption of LTNE conditions, our model contains three energy balances, coupled by so-called energy production terms.

In our previous contribution, we demonstrated that our model equations were in agreement with TPM-based models derived by others. We compared our model equations to TPM-based models also derived under LTNE conditions. In particular, we found that our energy balances, pressure relations and momentum balances were equivalent to theirs.

Summarised, we presented the model equations of our model, expected and agreed upon to be thermodynamically consistent a-priori. In particular, our model was derived obeying the principle of universal dissipation.

Contradicting this sentiment, we proceeded to demonstrate that our model elicits thermodynamically inconsistent behaviour under LTNE conditions. Specifically, terms which can only represent energy dissipation acted like a heat sink.

Since then, we have identified the root cause of this inconsistency.

The typically employed approach for model derivation within the TPM is the Coleman and Noll approach. Within this approach, an overall entropy inequality is constructed, terms are arranged meaningfully and each such term poses an entropy condition to be fulfilled.

The arrangement of terms is not unique. This is the root cause for thermodynamically inconsistent behaviour under LTNE conditions. In this contribution, we will demonstrate how to resolve this issue.

**Coupled Thermo-Hydro-Mechanical Modeling of Soil Freezing: Predicting Biot and Skempton Coefficients and Frost Heave Implications**

Williams Moises, Rodolfo Javier (1); Heider, Yousef (1); Meschke, Günther (2) 08:50
*1: Institute of Mechanics, University of Kassel, Kassel, Germany*
*2: Institute for Structural Mechanics, Ruhr University Bochum, Bochum, Germany*

In this contribution, we present a novel study on the coupled thermo-hydro-mechanical behavior of soils subjected to freezing under mechanical loading. The coupled response under undrained conditions is investigated through a numerical re-analysis of unique experimental tests that measure the variation of pore liquid pressure in response to a unit change in applied confining pressure for frozen soils [1]. This analysis is particularly relevant because the Skempton pore pressure coefficient plays a central role in capturing the coupled effects of pore fluid compressibility and solid skeleton compressibility in porous media, and it is a key parameter for investigating the definition of effective stress in frozen soils. To this end, we analyze advanced poromechanics theories that treat frozen soil as a three-phase material composed of soil grains, ice crystals, and unfrozen water, and the predicted

macroscopic coupling coefficients are compared with experimental measurements of the Skempton coefficient during freezing. Fully coupled formulations poromechanics of fully saturated freezing porous materials are considered, including thermo-hydro-mechanical model [2, 3], a thermo-hydro-mechanical phase-field models [4, 5], and a continuum micromechanics model, which allow identification of the Skempton coefficient based on theoretical assumptions. Preliminary results show that, using continuum micromechanics, the Skempton coefficient decreases with increasing ice saturation, consistent with experimental observations. Finally, we present a numerical application incorporating continuum micromechanics within a thermo-hydro-mechanical model [2, 3] to investigate implications for predicting frost heave in various soil types upon freezing.

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**A Theory of Porous Media–Extended Phase-Field Fracture Model for Saturated Soft Porous Materials**

Peters, Sven; Markert, Bernd 09:10
*Institute of General Mechanics (IAM), RWTH Aachen University, Germany*

Fracturing in soft, hydrated porous materials plays a crucial role in biomechanics, for example in biological tissues and hydrogels. The macroscopic prediction of crack nucleation and evolution under large deformations of the solid matrix remains a challenging task, particularly in soft hydrated materials where strong coupling between solid deformation and pore fluid pressure occurs. In hydrogels, for instance, this solid–fluid interaction under suitable loading conditions can lead to complex fracture phenomena, such as a stepwise advancement and arrest of cracks. This behavior is caused by consolidation effects at the crack tip.

To model this behavior, a macroscopic continuum mechanical approach based on the Theory of Porous Media (TPM) is developed. The proposed model accounts for both geometrical and material nonlinearities of the solid constituent. Crack initiation and propagation are described using a phase-field fracture (PFF) approach, in which crack topologies are approximated by a diffusive interface.

For the numerical treatment, the Finite Element Method (FEM) is employed for spatial discretization. A robust staggered solver is adopted, in which the poromechanical problem and the phase-field fracture problem are solved sequentially. The model is implemented within the FEniCSx framework.

**Potential method in the quasi-static problems of the coupled linear theory of elastic nanomaterials with triple porosity**

Mikelashvili, Mariam 09:30
*Ilia State University*

The paper focuses on the coupled linear quasi-static theory of elasticity for nanomaterials with triple porosity, incorporating concepts of Darcy's law and volume fractions of three levels of pores (macro-, meso-, and micropores). It formulates the general governing equations in terms of the displacement vector field, the changes of the pore volume fractions and fluid pressures in the pore networks for

three levels of pores. The fundamental three-dimensional boundary value problems (BVPs) describing steady vibrations in this theory are formulated and analyzed using the potential method, in particular, the boundary integral equation approach and the theory of singular integral equations.

Then, the surface and volume potentials, including single-layer and double-layer potentials, are constructed, and their basic properties are presented. Several useful singular integral operators are studied, and Noether theorems are established for these operators. The associated symbolic determinants and indices are computed explicitly.

Based on these results, the boundary value problems governing steady vibrations are transformed into equivalent systems of singular integral equations.

Finally, by means of the potential method (boundary integral equation method) and the theory of singular integral equations, existence theorems for classical solutions of all formulated BVPs are rigorously proved.

**Acknowledgments.** This work is supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG)[YS-24-148].

**Micro- to Nanoscale Metamaterials with Combined Flexo- and Piezoelectricity**

Kozinov, Sergey; Pham-Phu, Thuc; Balzani, Daniel 09:50
*Ruhr University Bochum, Germany*

Flexoelectricity and piezoelectricity provide two distinct mechanisms for electromechanical coupling: flexoelectricity arises from strain gradients and can occur in all dielectrics, whereas piezoelectricity is restricted to non-centrosymmetric materials and couples directly to strain. Architected microstructures (metamaterials) can be designed to induce strong local bending and strain gradients even under macroscopically uniform loading, thereby amplifying flexoelectric effects at micro- and nanoscales.
In this contribution, we present a numerical framework to investigate the combined piezo–flexoelectric response of dielectric metamaterials and to quantify the competition (or synergy) between intrinsic piezoelectricity and topology-induced flexoelectricity [1]. The model is based on an electric-enthalpy formulation that incorporates elasticity, strain-gradient elasticity (via a material length-scale parameter), dielectric response, and both linear (piezoelectric) and higher-order (flexoelectric) couplings. To avoid the C1-continuity requirement typical of strain-gradient theories, we employ a mixed finite element formulation with relaxed strain degrees of freedom and Lagrange-multiplier constraints.
Two representative architectures are studied: a dielectric strip with repeated triangular cutouts and a lattice design known to generate apparent piezoelectricity in centrosymmetric dielectrics. The formulation is first verified by reproducing characteristic electric-potential distributions and open-circuit voltage levels reported for purely flexoelectric metamaterial designs. We then perform systematic parameter studies varying geometric size and the strain-gradient length scale, and compare purely flexoelectric, purely piezoelectric, and combined piezo–flexoelectric material behaviors.
Results reveal a clear size-dependent transition: flexoelectricity dominates at sufficiently small feature sizes, while piezoelectricity prevails at larger scales. Depending on architecture and deformation mode, the interaction can either enhance or suppress the net electrical output, and even lead to sign changes in the open-circuit potential for certain lattices. These findings provide design guidelines for tailoring geometry and length scales in next-generation micro-/nanoscale sensors and energy harvesters, and motivate targeted experimental fabrication routes (e.g., high-resolution additive manufacturing) for validating the predicted trends.
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**Thermo-Mechanical Effects on Reflection Characteristics of Meta-Materials for mm-Wave Applications in the Outdoor Environment**

Gomez, Roshan; Kaliske, Michael
*Technische Universität Dresden, Germany*

10:10

Safe and reliable communication infrastructure for advanced air mobility (AAM) requires an intelligent and adaptable propagation channel. Electromagnetic (EM) meta-materials and meta-surfaces such as the reconfigurable intelligent surface (RIS) enable such intelligence allowing programmability with multiple modes of EM wave manipulation. Current literature on RIS and other radio-frequency meta-materials show focused engineering efforts towards the design and indoor experimental testing of RIS for mm-Wave applications.
Although crucial for practical implementation, physical studies on the effects of the varying environmental conditions such as temperature, moisture, wind and strains of the host surface on the EM response of these devices are limited by the high costs of planning, frequency band licensing and outdoor environment emulators. From the simulation perspective, high-frequency asymptotic methods such as ray-tracing (RT) are being used for the computation of radio coverage maps including RIS, which are inherently incapable of taking multi-physics effects int account.
As the first step to address these challenges, we develop a thermo-mechanical finite element (FE) co-simulation of EM scattering to compute the EM near-field. A thermo-mechanical simulation of a meta-surface device deforms the mesh to be used for an EM scattering simulation. For the FE scattering model, Bloch-periodic boundary conditions and perfectly matched layers (PML) are used to truncate the scattering domain, which is discretized by Nedelec elements.
Far-field parameters may be computed from this framework using near-to-far-field transformations (NFFTs) and used directly in ray-tracing simulators to generate radio coverage maps. These are highly beneficial for the planning and resource-aware operation of meta-material augmented communication networks. Moreover, the physics-aware scattering simulation may be used for the design of meta-surfaces to be durable and to show consistent long-term performance in an outdoor environment.

## S07.07: Chemo-/thermo-/hygro-/electro/-mechanical coupling

Date: March 19, 2026 14:00–16:00
Room: KII, M17.02
Chair(s): Böhlke, Thomas

**Electro-chemo-mechanical modeling of structural battery electrode materials with focus on processes at material interfaces**

Rollin, David (1); Larsson, Fredrik (2); Runesson, Kenneth (2); Jänicke, Ralf (1)
*1: TU Braunschweig, Germany*
*2: Chalmers University of Technology, Sweden*

14:00

Li-ion batteries are a crucial component of various systems. For some of them, e.g. electric vehicles, reducing the mass and volume of the batteries is an important aspect for optimizing the overall performance. One approach uses structural batteries combining load bearing and battery functionality in a single composite material.

There are different designs of structural batteries. One of them is based on multi-functional properties of carbon fibers, employing them as electron transport medium, mechanical reinforcement and Lithium storage in the negative electrode. The storage material in the positive electrode is incorporated as particles in a coating on the carbon fibers. These particles are connected by a porous binder matrix. The pore space is filled with an electrolyte for Li-ion transport. Our aim is to develop a model describing the electro-chemo-mechanical coupling mechanisms in such a type of microstructure.

A complete model of all relevant processes would be highly nonlinear and include complex aspects like large deformations, damage and non-standard diffusive transport. However, as a manageable intermediate step, we focus on capturing the processes at the interfaces between the different phases. Accounting for jumps in the primary fields at the interfaces requires modeling constitutive relations for the corresponding fluxes across the interfaces. For the bulk phases, we consider small strain kinematics, linear-elastic quasi-static deformation, linear diffusion, electro-statics and linear couplings between the electro-chemical and mechanical processes. Nonlinear constitutive relations are considered for the chemical potential inside the bulk material and the reaction kinetics at the particle-electrolyte interface.

In the future, we aim to use this model as the basis for a multi-scale approach employing the concept of variationally consistent homogenization. This way, an effective macro-scale model and an upscaling procedure from a representative volume element can be derived to gain understanding of the effective behavior of the system and pave the way towards a model of a whole battery.

**Electro-Chemo-Hydro-Mechanical Modeling of PEMWE Anode Catalyst Layers: The Role of Phase Change in Partially Saturated Porous Media**

Sidharth, PC (1); Antonini, Alberto (1); Rao, B. N. (2); Aldakheel, Fadi (1) 14:20
*1: Leibniz University Hannover, Germany*
*2: Indian Institute of Technology Madras, Chennai, India*

Proton Exchange Membrane Water Electrolysis (PEMWE) stands at the forefront of sustainable Green Hydrogen production, offering a vital pathway for decarbonizing heavy industries and storing intermittent renewable energy. However, the widespread commercialization of this technology is currently constrained by the efficiency and durability of the Anode Catalyst Layer (aCL). As the site of the Oxygen Evolution Reaction (OER), the aCL operates under complex multiphysics interactions. Optimizing this component is severely impeded by critical limitations in state-of-the-art computational modeling. Prevalent one-dimensional (1D) models inherently fail to capture the lateral heterogeneities in stress and mass transport caused by the geometry of the Porous Transport Layer (PTL). Furthermore, standard approaches frequently neglect the mechanical compression of the cell assembly and simplify the pore gas to pure oxygen. At high current densities, ignoring water-to-vapour phase change kinetics leads to a drastic underestimation of the gas volume fraction, thereby failing to predict the onset of anode dry-out events.

To resolve these complexities, this work utilizes the thermodynamic framework of the Theory of Porous Media (TPM) to develop a fully coupled electro-chemo-hydro-mechanical model of the aCL. This framework allows for the explicit resolution of lateral transport pathways and mechanical stress concentrations. Furthermore, the mass balance equations are extended to treat the gas phase as a binary mixture of oxygen and water vapour. Unlike simplified equilibrium models, this work incorporates explicit evaporation and condensation source terms to dynamically track the transition from liquid-saturated operation to vapour-induced pore blockage. This formulation captures the critical competition between capillary liquid supply and the rapid volumetric expansion of water vapour, allowing for the precise prediction of localized dry-out events where the accumulating gas phase physically displaces the liquid reactant.

Numerical results demonstrate that the complex interplay between phase change, mechanical deformation, and transport limitations critically governs cell performance, providing essential guidelines for optimizing next-generation electrolyzer designs.

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**From Microstructure to Performance: A Multiscale Multiphysics Model of Solid Oxide Fuel Cells**

Langner, Eric; Semenov, Artem; Wallmersperger, Thomas 14:40
*Institute of Solid Mechanics, TU Dresden, Germany*

Solid oxide fuel cells (SOFCs) are promising energy converters that can help to reduce anthropogenic carbon dioxide emissions. However, technical issues such as electrochemical degradation and mechanical cracking require a better understanding of the individual layers of the structures and how they interact [1]. In the present research, a multiscale and multiphysics modeling approach is given to capture the effect of the porous anodes on the macroscopic performance. First, the morphology of the electrode is characterized using morphological descriptors, and the effective properties (i.e., the transport and mechanical properties) are computed by the first-order homogenization method [2]. Second, the properties are incorporated into a multiphysical macroscopic model. This model includes electrical, chemical, thermal, and mechanical fields to obtain key performance indicators, such as the electric power density of a single cell. Since SOFCs operate at high temperatures, the model also considers the effective creep properties [3]. The present research creates a sophisticated structure-property-performance simulation chain as a basis for optimizing the microstructure of individual fuel cell layers.

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**Generating short-fiber reinforced polymer microstructure with Fiber-length and Fiber-orientation coupling**

Mehta, Alok Ranjit; Schneider, Matti 15:00
*University of Duisburg-Essen, Germany*

To compute effective mechanical properties of injection molded Short-Fiber Reinforced Polymers (SFRP) using computational homogenization, it is required to create a Representative Volume Element (RVE) which contains all relevant statistical information such as fiber-length distribution, fiber-orientation distribution, volume fraction of constituents, spatial arrangement of constituents etc. Although all this information is necessary, the RVE should be as small as possible to be computationally efficient. These contradicting demands require careful consideration of all the parameters involved.

In reality for injection molded SFRP components, the fiber-lengths and the fiber-orientations are dependent on each other [1]. In other words, by changing the fiber-length distribution function, the fiber

orientation distribution function changes. There has been work on this particular behavior which involves finding an maximum of a information-theoretic entropy [2]. In this work we propose an alternative approach.

We discuss the critical components of the developed model and present the computed effective properties for the same. We also validate our results with experimental data.

**References**

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**Thermo-Mechanical Modeling of Paper and Paperboard**

Jellen, Finnja; Kopic-Osmanovic, Nadir; Simon, Jaan-Willem 15:20
*University of Wuppertal, Germany*

Paper and paperboard are materials of particular relevance in the packaging industry due to their resource-efficient and versatile properties. However, their anisotropic temperature dependent elastic–plastic behavior makes phenomenological modeling challenging. Nevertheless, coupling the mechanical and thermal behavior is especially important for predicting and optimizing industrial forming processes at elevated temperatures, and for reducing trial-and-error experimentation. Therefore, a thermo-mechanically coupled anisotropic elasto-plastic material model for paper and paperboard was developed. It was formulated in a thermodynamically consistent manner and valid for large deformations. For plasticity modeling, the yield function proposed by Kopic-Osmanovic et al.[1] was chosen to accurately represent the material's anisotropic behavior. To capture the anisotropy arising from the microstructure, the concept of structural tensors was applied. A covariant mapping of the structural tensors was used for the in-plane components, and a contravariant mapping for the out-of-plane components. As a consequence, the in-plane structural vectors were allowed to change their orientation during plastic deformation, whereas the out-of-plane vector remained orthogonal to the in-plane directions. All relevant quantities were mapped into the co-rotated intermediate configuration, instead of the intermediate configuration, to avoid the pull-back operations to the reference configuration. Regarding the thermo-mechanical modeling, the model accounted for heat generation due to plastic deformation, while temperature changes induced anisotropic thermal expansion and a decrease in stiffness and strength. Therefore, the free energy was formulated by decomposing it into an area-changing and an isoplanar contribution and incorporated thermo-mechanical coupling terms. Furthermore, heat conduction was treated anisotropically. The implementation was carried out in FEniCS using FEMExternalOperator and JAX for the algorithmic treatment of plasticity and for automatic differentiation. To validate the framework, both integration-point studies and structural examples under combined thermo-mechanical loading were performed. These examples examined temperature-dependent material behavior, heat generation from plastic deformation and anisotropic heat flux in in-plane and out-of-plane directions. All in all, the industry continues to face inefficiencies and increased material waste in various forming processes due to the lack of accurate models describing the mechanical and thermal behavior of paper and paperboard. The presented model therefore offers a promising solution to reduce such material losses by enabling more reliable predictions and optimized process control.

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**Thermo-Mechanical Response of LiAlO2 Subjected to Laminar Strained Premixed Flames based on coupled modeling approach**

Yu, Chunkan (1); Hille, Frederik (2); Li, Chenglin (1); Böhlke, Thomas (2); Fischlschweiger, Michael (1) 15:40

*1: Institute of Technical Thermodynamics, Karlsruhe Institute of Technology (KIT), Germany*
*2: Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Germany*

This work investigates the coupled flame–material interaction that develops when a laminar strained premixed methane/hydrogen/air flame impinges on and heats a $LiAlO_2$ plate. The central objective is to quantify how reactive-flow conditions interact with solid material to determine the transient thermo-mechanical response of high-temperature structural materials. The material behavior is modeled using linear thermoelasticity, enabling prediction of time-dependent deformation, temperature evolution, and the response of flame-induced thermo-mechanical stresses arising from steep flame-induced temperature gradients.

On the combustion side, the strained premixed flame is simulated using a detailed molecular transport model that incorporates multicomponent diffusion, species-dependent differential diffusion, and thermal diffusion (Soret) effects. These transport mechanisms are combined with detailed chemical kinetics to accurately resolve the flame structure and dynamics. Heterogeneous surface reactions describing the destruction of reactive radicals at the solid surface are also included.

The thermal interaction between gas-phase and solid-phase domains is described using a conjugate heat-transfer framework, within which the gas temperature, interfacial heat flux, and internal solid temperature field are solved in a fully consistent manner. Parametric variations of flame conditions including hydrogen enrichment in the unburnt mixture and changes in the imposed strain rate are examined to determine their influence on surface heating, internal thermal gradients, and the resulting thermo-mechanical stress development.

Two metrics of material integrity are evaluated: the time required for the maximum thermoelastic stress to reach the yield strength, and the time for the material temperature to approach its melting temperature. The analysis shows how reactive-flow parameters, fuel composition, and flame strain rate influence both the magnitude and temporal rate of thermo-mechanical loading. These results clarify how low-carbon combustion strategies, such as hydrogen addition, can either mitigate or intensify material degradation. The findings provide guidance for designing flame-exposed components and underscore the importance of coupled reactive-flow and thermo-mechanical modeling for predicting material limits under high-temperature reactive environments.

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**S07.09: Thermo-mechanical processes & manufacturing**

Date: March 20, 2026 08:30–10:30
Room: KII, M17.02
Chair(s): Wallmersperger, Thomas

**An Enhanced Phase-Dependent Thermo-Mechanical model for Metal Powder Bed Fusion**

Noll, Isabelle (1,2); Remmers, Joris (2); Menzel, Andreas (1,3) 08:30

*1: TU Dortmund University, Germany*
*2: Eindhoven University of Technology, The Netherlands*
*3: Lund University, Sweden*

Additive manufacturing (AM) of metals, particularly laser powder bed fusion (PBF/LB-M), involves extreme thermal gradients, rapid phase changes, and strong thermo-mechanical coupling across multiple spatial and temporal scales. Reliable material models and numerical simulations are essential for understanding deformation and residual stress development, as well as for systematically investigating the influence of process parameters and physical mechanisms, thereby enabling process optimization, laser beam shaping strategies, and the accelerated development of new alloy for manufacturing.

This contribution present a fully coupled and phase-dependent finite element (FE) framework for modelling the effective behaviour of metals during PBF-LB/M. The framework explicitly resolves powder-melt-solid transitions by using different constitutive material models as well as phase specific temperature-dependent material properties. The thermal model accounts for conduction, convection, radiation, and evaporation-induced heat loss, and incorporates latent heat effects and internal heat generation consistently. Mechanical effects, such as transformation strains and stress relaxation, are considered, which are important during phase transitions, enabling realistic prediction of stress evolution and deformation.

The governing equations form an overall strongly coupled non-linear system, which is solved monolithically using an in-house FE framework. Surface and bulk elements are treated separately in order to capture phase- and temperature-dependent boundary effects, as well as evolving domains using a stress-free layer activation strategy to represent material addition.

Numerical examples demonstrate the impact of phase transitions and thermo-mechanical coupling on temperature evolution, melt pool geometry, and stress development. The results emphasise the importance of rigorous physically motivated formulations in capturing key PBF/LB-M phenomena on a continuum scale and form the basis for further methodological development.

**Radiative Transfer Model for Laser-Powder Interaction in Directed Energy Deposition**

Puthoor, Alfred Jose; de Payrebrune, Kristin 08:50

*RPTU Kaiserslautern-Landau, Germany*

Laser-based metal additive manufacturing enables fabrication of complex three-dimensional components by melting metal powders layer-by-layer. When a high-power laser beam interacts with metal powder particles, energy is absorbed through multiple scattering and absorption events, a process governed by radiative transfer theory. Accurate prediction of how much laser energy is absorbed, and where this energy is deposited spatially, is essential for controlling the additive manufacturing process [1,2]. In laser directed energy deposition (L-DED), metal powder is injected directly into the laser beam as a stream of particles suspended in an inert gas. This creates a unique challenge: the powder concentration is extremely low compared to conventional powder bed processes, resulting in fundamentally different laser-powder interaction physics. Existing radiative transfer models were developed for densely packed powder beds where particles are close enough that their scattered light fields interfere with each other (dependent scattering) [3,4]. However, in the less dense L-DED environment, particles scatter light independently, and the dominant physics shifts from surface-based absorption to volumetric absorption distributed over millimeter-scale distances. Current models either oversimplify this physics using empirical fitting parameters [5,6], or rely on computationally expensive particle-by-particle ray tracing simulations that are impractical for process optimization [7,8].

This work addresses the gap of computationally efficient, physics-based models for volumetric absorption in less dense powder streams by developing a model for laser-powder interaction in L-DED. Starting from the radiative transfer equation, the fundamental law governing photon transport through scattering media, we demonstrate that the high porosity of L-DED powder streams enables a simplified one-flux formulation where backward-scattered radiation is negligible. This yields closed-form analytical expressions for the absorbed power distribution that can be evaluated efficiently compared to traditional approaches [3,4]. The model accounts for three-dimensional spatial variations in powder concentration validated using experimental imaging. This method enables integration with thermal-mechanical simulation frameworks for predicting temperature gradients and residual stresses, providing a foundation for physics-based process simulation for L-DED.

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**Rheological Characterization of Solid Hydrogel Laminates**

Güneş, Gönç Berk (1,2); Fauser, Dominik (1,2); Kim, Semi (3); Ludwigs, Sabine (3); Steeb, Holger (1,2)

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*2: Stuttgart Center for Simulation Science (SC SimTech), University of Stuttgart, Pfaffenwaldring 5a, Stuttgart, D-70569, Germany*

*3: Institute of Polymer Chemistry, University of Stuttgart, Pfaffenwaldring 55, Stuttgart, D-70569, Germany*

09:10

Various plants, like pinecones or resurrection plants show humidity-driven shape morphing behavior without the need for active control or external power. In these systems, complex shape changes are possible due to combination of different contrary or anisotropy material behavior. Inspired by nature, functional polymers, like solid hydrogels are capable of changing their shape and mechanical behavior in response to external stimuli like heat and moisture.

In this work, the focus is on establishing a fundamental understanding of how the hydrogels respond to environmental stimuli. To investigate how humidity and temperature couple with the time-dependent mechanics of solid hydrogels, we perform uniaxial extensional oscillatory tests on homogenous isotropic samples in a stress-controlled configuration (allowing the samples to swell during measurement). All tests are conducted within the linear viscoelastic (LVE) range, with amplitude sweeps used to determine admissible strain amplitudes. Frequency sweeps are carried out at constant temperature and at equilibrium water content to characterize how internal hydration interacts with viscoelastic behavior under free swelling. Complementarily, temperature sweeps at constant amplitude, frequency and relative humidity are performed to isolate the influence of temperature on

the moisture and time-dependent material behavior. Together, these measurements reveal how humidity and temperature affect both the complex modulus and the axial strain. For further extending the understanding of these complex material settings, measured axial thermal and moisture strain is used to calculate the pure volumetric thermal and moisture strain by assuming incompressible material behavior.

To develop complex shape changing structures as observed in nature, we developed a method to 3D print solid hydrogel samples. This procedure fabricates anisotropic structures which influences the shape-morphing behavior. For understanding the influence of anisotropic structure on the shape-morphing behavior, same coupled rheological measurements are carried on 3D printed samples and compared with homogenous ones.

These insights provide a basis for translating the material behavior into controllable macroscopic shape changes, forming a foundation for future 4D-printing strategies.

**Coupled Mass–Momentum Formulation of Wear for Contact Problems**

El Masri, Samir; Antuna Uzeda, Sergio Andres; Storm, Johannes; Kaliske, Michael
*Technische Universität Dresden, Germany*

09:30

The finite element method (FEM) provides a mature framework for solid deformation; however, surface deteriorative processes in solids remain insufficiently addressed. Wear highlights this gap, as it has yet to see a practical continuum mechanics FEM application. Moreover, the continuum mechanics of wear remains underdeveloped, with most existing approaches relying on empirical or decoupled formulations that fail to capture the coupling between contact and material loss. When a body undergoes contact, wear-induced mass loss naturally necessitates treating the system as an open one, requiring a consistent treatment of mass removal and its influence on the mechanical response.
To address this gap, a framework that incorporates wear directly into the continuum description is introduced, enabling a physically meaningful coupling between the mass and momentum balance. The governing equations are extended by introducing a wear field as an additional degree of freedom and formulating the mass and momentum balance in a fully coupled manner. A consistent finite element implementation is developed to solve the complete system in a fully monolithic way, ensuring a coupled interaction between wear and deformation. Numerical challenges arising from mass loss and contact are addressed through appropriate stabilization and contact treatment. Finally, through a series of examples, the monolithic method is compared with existing wear modelling approaches, demonstrating improved accuracy and robustness.

**Solution algorithms for the numerical treatment of strain-gradient crystal plasticity**

Lara, Jose; Steinmann, Paul
*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

09:50

Classic plasticity theories are not able to reproduce the size-dependent material behavior observed in metals, namely, smaller is stronger. Strain-gradient formulations introduce an intrinsic material length scale, enabling the capture of such size effects. Gurtin's crystal plasticity framework achieves this by considering the plastic slips and their gradients as state variables and introducing a microforce and microstress pair as their respective energetic conjugate. This yields the standard linear momentum balance together with a pseudo-balance per slip system, which can be seen as the nonlocal yield condition of the respective slip system. The discretization of the governing equations form a saddle-point problem, which motive the exploration of alternative solution strategies to the monolithic approach. Two staggered algorithms are presented and numerically implemented to successfully solve the simple shear of a infinite strip. The algorithms' performance is analyzed and compared to the monolithic approach.

**Inferring the Constitutive Behavior of Additively Manufactured Aluminum through Micro Compression Testing and Finite Element Modeling**

Burkart, Klaus; Farhat, Malik; Toenjes, Anastasiya; Eisenträger, Johanna 10:10
*Leibniz-Institut für Werkstofforientierte Technologien – IWT / Leibniz Institute for Materials Engineering – IWT, Bremen, Germany*

Additive manufacturing (AM) enables near-net-shape production of components with complex geometries, but the resulting mechanical properties depend strongly on local dimensions and cross-sectional variations. These scaling effects become evident during fabrication as well as during mechanical testing. Micro compression testing has emerged as a sensitive, high-throughput method for characterizing the elasto-plastic cyclic response of additively manufactured mini-cylinders while requiring only minimal material and allowing specimens to remain on the build plate.

In this contribution, we present a constitutive modeling approach for predicting the mechanical behavior of additively manufactured aluminum, informed by micro compression experiments and nonlinear finite element simulations. We manufacture samples of different sizes on a single build plate to systematically capture scaling effects and to relate micro compression data to the behavior observed in conventional mechanical tests. We investigate how various constitutive models for aluminum under cyclic loading — covering elastic, plastic, and inelastic mechanisms — affect the simulated micro-compression response.

Our finite element framework includes detailed contact modeling between the indenter and specimen surface as well as the lateral constraint imposed by on-plate fixation. By correlating experimental measurements with simulated results, we demonstrate how micro compression testing can be used to infer the actual constitutive behavior of additively manufactured aluminum. The contribution highlights the mechanical insights gained from combining tailored constitutive modeling with size-dependent testing at the microscale. The derived constitutive laws form a critical input for subsequent fracture mechanics-based models that are used to predict the fatigue limit of AM components.

## S07.09.2: Fluid-structure interaction

Date: March 20, 2026 08:30–10:30
Room: KII, M17.52
Chair(s): Schulte, Miriam

**Topology optimization using the finite cell method for vibroacoustic problems in the time domain**

Radtke, Lars (1); Eisenträger, Sascha (2); Düster, Alexander (3) 08:30
*1: University of Rostock, Germany*
*2: Otto von Guericke University, Germany*
*3: Hamburg University of Technology, Germany*

This work combines recent advances in the finite cell method (FCM) for transient problems with a topology optimization framework based on level-set representations, modern shape update concepts, and the continuous adjoint method. The focus is on coupled vibroacoustics, where transient structural vibrations interact with acoustic wave propagation. Solid and fluid domains are discretized by two superimposed FCM discretizations, enabling a unified treatment of complex geometries without boundary-fitted meshes. The interaction is modeled using a monolithic Neumann-Neumann coupling approach.

The FCM is an immersed boundary method that employs high-order finite elements together with tailored quadrature rules and stabilization techniques for cut elements. This yields an accuracy comparable to classical high-order finite element methods and allows to use explicit time integration schemes with comparably large critical time step sizes.

**Coupling Scaled Boundary Perfectly Matched Layers with Immersed Vibroacoustics**

Jambagi, Mahendra Bhimappa (1); Zhang, Junru (3); Zhang, Junqi (3); Eisenträger, Sascha (2); Radtke, Lars (1)

*1: Chair of Structural Mechanics, Universtiy of Rostock, Germany*
*2: Chair of Computational Mechanics, Otto von Guericke University Magdeburg, Germany*
*3: Key Laboratory of Urban Security and Disaster Engineering of Ministry of Education, Beijing University of Technology, Beijing , China*

08:50

Accurate time-domain simulation of vibroacoustic wave propagation requires efficient absorbing boundary conditions, particularly for high-frequency and longtime analyses. This paper presents a scaled boundary perfectly matched layer (SBPML) formulation integrated into a finite cell method (FCM) framework for vibroacoustic problems. The approach combines scaled boundary coordinates with complex coordinate stretching to achieve effective absorption at the boundaries of the acoustic domain within a fictitious domain setting. Structural dynamics and acoustic wave propagation are coupled in the time domain and discretized using the finite cell method. The performance of the proposed method is demonstrated through numerical examples of wave propagation, with absorption efficiency and stability are evaluated using pressure fields, particle velocities, and transmitted acoustic energy. Frequency-domain characteristics are further analyzed via Fourier transforms of time-domain responses, confirming the effectiveness of the SBPML–FCM approach for vibroacoustic simulations.

**Partitioned Fluid-Structure Interaction in Maritime Applications**

Kühne, Christian; Düster, Alexander

*Numerical Structural Analysis with Application in Ship Technology (M-10), Hamburg University of Technology, Germany*

09:10

Numerical simulations are essential for designing maritime systems, such as ocean energy harvesting devices, floating wind turbines, ship propellers, or wind-assisted propulsion systems. Accurately capturing the complex behavior of these devices requires addressing multi-field problems, specifically the Fluid-Structure Interaction (FSI). To solve these problems, we employ a partitioned coupling approach which allows for the utilization of existing specialized solvers for each domain.

In this presentation, we focus on the partitioned coupling techniques implemented within our in-house software, comana (König et al., 2016). Efficient partitioned coupling requires addressing specific challenges, such as accelerating the coupling iteration and performing reliable interpolations between the different computational domains. In addition, the computational cost of the individual solvers must be considered to ensure a fast solution to the coupled problem. We illustrate the modeling and simulation method by applying it to different maritime applications. Furthermore, we present a comparison between three-dimensional high-order solid elements (Düster et al., 2017) and traditional shell elements to discretize the thin-walled structure.

References:

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**Higher-order block-structured meshing for moving domains with connectivity changes**

Schalk, Teresa; Fries, Thomas-Peter 09:30
*Graz University of Technology, Austria*

We present a novel block-structured mesh generation and re-generation method, applicable for any type of domain movement, even with topology or connectivity changes. By coarsely partitioning the domain into blocks, herein, represented by coarse, linear quads, a block-structure is generated and each block may be meshed individually. Different block-structures are used during a simulation, each tailored to the occurring domain geometry. The exact geometry and possible grading information is assigned to the blocks, which enables the generation of (higher-order) meshes throughout the simulation [1, 2, 4]. The change between different block-structures is a delicate task and has possible consequences on the handling of the governing equations. Data projection between the corresponding computational meshes is required, nevertheless, this is done rarely and may be restricted to local regions of the domain. Herein, we focus on incompressible flow simulations that include moving domains, with large translations and rotations. For the Navier-Stokes equations, an Arbitrary Lagrangian-Eulerian formulation with Taylor-Hood elements is used. For the temporal discretization we suggest the Crank-Nicolson method, whereas, the pressure is treated fully implicit [3], to avoid any oscillations after the projection. Numerical results, including a flow through a rotary lobe pump and moving flaps in a channel flow, confirm the success of the presented approach.

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**Aeroelastic finite element modelling of slender rotating blades**

Bassetti, Alessandro 09:50
*Hamburg University of Technology, Germany*

The aeroelastic dynamics of a slender rotor blade is modelled by using 1-D finite elements. The elements are arbitrarily oriented in the hub reference system, allowing the description of blades with curvilinear axis. The aerodynamic and inertial loading on the elements depend on the deformation of the element, whose elementary section is assumed to move with displacements and rotations in the 3-dimensional space. Given a set of configurations with varying collective pitch and precone angles of the blade root in a hovering state with a specific rotation speed of the hub, the discretised blade is allowed to deform into a stationary equilibrium according to the steady aerodynamic and centrifugal loads. The flutter stability is then assessed for small perturbations of the stationary equilibrium. Here the unsteady aerodynamic loads are limited to the quasi-stationary component and do not include the effects of the wake dynamics.

**A Coupled Definition of Jet Engine Thrust and Aircraft Drag**

Yuan, Yiwen; Staudacher, Stephan; Zabel, Myles; Weigand, Bernhard 10:10
*University of Stuttgart, Germany*

The thrust force of a jet engine arises from the pressure and frictional forces on the gas path surfaces such as blades, vanes, casings and ducts. Being difficult to compute on this level of detail, the change of the momentum flux entering and exiting the engine is typically used to derive the thrust force as an integral value. Whilst being simple to apply for an engine installation which is unaffected by the aircraft flow, this concept comes to a limit in more complex installation.

Starting with the basic equation for the pressure and frictional forces on the gas path surfaces, we show the derivation of the jet engine thrust force for today's forms of engine under-wing installation. We discuss the consequence for the definition of aircraft drag and its dependence on engine and aircraft operating conditions.

In a second step, we introduce the concept of thrust defined with an integrated control volume and its consequence for highly integrated jet engines. We demonstrate that this definition links parts of the aircraft drag to engine thrust and vice versa. As a consequence, the accounting of aircraft drag and engine thrust becomes dependent on the engine operating point and the flight conditions. Understanding this relationship makes this type of drag and thrust accounting directly applicable to aircraft mission assessment.

In a third step, we introduce the concept of the power balance method to assess overall aircraft efficiency. We show how the engine gas path flow conditions act as boundary conditions to the aircraft power balance method which gives rise to the so-called truncated control volume thrust definition. This leaves space to carefully define the boundaries of the engine as a system.

It turns out, that the definition of engine thrust not only depends on the engine installation but also on the method used to evaluate aircraft performance.

## S08: Multiscales and homogenization

Organizer(s): Klinge, Sandra *(Technische Universität Berlin)*
Eisenträger, Johanna *(Leibniz Institute for Materials Engineering - IWT)*

## S08.01: Metamaterials and Additive Manufacturing

Date: March 17, 2026 08:30–10:30
Room: KI, M11.42
Chair(s): Schneider, Matti
Warkentin, Andreas

### Static Size Effects and Wave Scattering in Mechanical Metamaterials: A Relaxed Micromorphic Perspective

Sarhil, Mohammad; Madeo, Angela 08:30
*Lehrstuhl Baumechanik, Institut für Baumechanik, Statik und Dynamik, TU Dortmund, Germany*

Mechanical metamaterials exhibit distinctive phenomena such as size effects under static loading and the presence of band gaps, i.e., frequency ranges in which wave propagation is inhibited. In this talk, we investigate the interplay between static size effects and the dynamic scattering behavior of mechanical metamaterials. To this end, a two-stage optimization procedure is proposed to identify the material parameters of the relaxed micromorphic model (RMM).

The RMM is subsequently implemented in targeted finite element simulations and systematically compared with fully resolved microstructured simulations to assess the influence of curvature terms in metamaterials of finite size. The results demonstrate that curvature effects play a significant role in both the static and dynamic regimes, highlighting their importance for accurately capturing size-dependent responses and wave propagation phenomena in mechanical metamaterials.

### Computational Homogenization and Data-Driven Constitutive Laws for Graded Architected Materials

Frey, Moritz; Brandstaeter, Sebastian; Popp, Alexander 08:50
*University of the Bundeswehr Munich, Germany*

Mechanical metamaterials derive their macroscopic behavior from the mechanics of their microstructure rather than from the base materials themselves. Their resulting properties are determined by the geometry and interactions of the design elements. Controlling these microstructural features opens new possibilities for applications in adaptive structures, impact absorption, and programmable stiffness materials.

This talk explores the design of unit cells with self-contact mechanisms to achieve mechanical metamaterials with programmable, progressive stiffness properties. Particular emphasis is placed on graded architectured materials, where spatially varying geometric properties such as internal contact surfaces enable location-dependent mechanical responses. Using nonlinear finite element models from computational contact mechanics, we demonstrate how spatial variation in microstructural parameters enables tuning of macroscopic stiffness fields.

To address the computational cost associated with modeling such systems, we consider data-driven constitutive approaches as alternatives to multiscale schemes such as $FE^2$, which quickly become prohibitively expensive for more complex metamaterials. In this context, we assess data-driven constitutive models for predicting the mechanical behavior of unit cells with contact interactions and spatially varying design parameters. These models incorporate stress–strain data together with geometric and spatial parameters of the microstructure, providing a basis for efficient homogenization.

**Multiscale Optimization of Beam-Based Microstructures for Programmable Mechanical Behavior**

Alkafri, Banan (1); Leichner, Alexander (1); Simeon, Bernd (2)
*1: Fraunhofer ITWM, Kaiserslautern*
*2: Fachbereich Mathematik, RPTU Kaiserslautern*

09:10

Programmable metamaterials are of a rising interest in many real-world applications. These materials consist of array of periodic unit cells, often referred to as microstructures. By adjusting the geometry of these microstructures, programmable metamaterials can be tailored to achieve certain mechanical behavior. To design such materials, previous work [1,2] proposed a multi-scale framework in which the macroscopic response of the material can be controlled through a set of design parameters that defines the geometry of each unit cell.

In this framework, an optimization problem is formulated, and the design parameters serve as control variables so that the desired macroscopic response is achieved. The optimization problem is then solved using an adjoint based method, which provides the gradient for updating the design parameters iteratively using gradient decent until the desired macroscopic behavior is achieved. While topology optimization changes the topology by adding or removing material, the proposed framework fixes the microstructure topology and optimizes its geometric parameters, so that the macroscopic behavior can be programmed.

However, the framework is limited to specific microstructure designs and specific cost functional. Our work extends this framework to include microstructures that are designed using beams. As a first step, we generated various beam-based unit cells and assigned design parameters to those cells such as beam thickness, base length, and beam height. Later steps include studying their mechanical behavior under various loading conditions such as compression and tension, in order to understand the effect of the parameters on the overall behavior of the unit cell. Building on this, later stages include extending the optimization framework. This can be done by including different types of cost functionals such as tracking stresses or internal variables to achieve stable solution of the adjoint problem. In addition, inclusion of more constraints like volume limits will be considered. These extensions aim to make the framework more capable of achieving more complex material behavior, which leads to more stable approach for designing microstructures with targeted mechanical properties.

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[2] T. Lichti, *Development of Methods and Tools for the Design of Programmable Materials*, PhD Thesis, Fraunhofer Verlag, 2024.

**A voxel-based homogenization framework for additive manufactured materials**

Hellebrand, Sonja (1); Brands, Dominik (1); Xu, Bai-Xiang (2); Schröder, Jörg (1)
*1: University of Duisburg-Essen, Germany*
*2: TU Darmstadt, Germany*

09:30

Additive manufacturing (AM) is becoming increasingly popular in the field of industrial design for creating complex geometries that would be difficult or impossible to produce using traditional manufacturing methods. Instead, AM allows to fabricate components without assembling junctures, enabling more integrated and optimized designs that reduce weight and improve performance. One widely used method in AM is laser powder bed fusion with selective sintering.
Despite the significant advantages of AM, one limitation is the porosity of the resulting material, which arises due to incomplete fusion or gas entrapment, for instance. These pores, which can vary in size, shape, and distribution, have a critical impact on the mechanical properties of the final component. Understanding and controlling porosity is therefore essential for ensuring the reliability and performance of parts produced by additive manufacturing.

This motivates to focus on the computational modeling and analysis of porous microstructures produced by selective sintering, [1]. Three-dimensional voxel data, which represent the material distribution within the porous microstructure, are used as the basis for generating finite element meshes. These meshes of different resolution and refinement allow a detailed numerical investigation of the mechanical behavior of the material at the microscale.
A key aspect in the analysis of the mechanical properties of microstructures are the effective properties, which reflect the macroscopic behavior of the materials, [2] on their computational treatment. By systematically varying key process parameters, such as laser power and laser scan speed, their influence on the effective mechanical properties of the porous structures are examined. In this contribution, these effective properties are determined by numerical homogenization, which result in large systems of equations ($\tilde{1}0^8$ dofs), which are successfully solved utilizing high performance computing tools. The results and findings can be used in many ways to increase the efficiency of numerical simulations. Both for generating statistically similar representative volume elements, [3], and as a training data set for teaching artificial intelligence models.

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**Computational investigation of anisotropic sand-binder microstructures**

Alatassi, Talat (1); Jabs, Lukas (1); Donval, Elodie (2); Schneider, Matti (1,3)
*1: University of Duisburg-Essen, Germany*
*2: Univ. Grenoble Alpes, CNRS, Grenoble INP, 3SR, 38000 Grenoble, France*
*3: Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern*

09:50

To obtain suitable microstructures for micromechanical investigations without relying on slow and expensive physical test specimens, geometric descriptions of microstructures have proven advantageous, because they offer immediate control over the parameters that characterize the microstructures. One example of industrial relevance is 3D-printed sand cores for casting applications. These cores must meet various requirements, some of which are conflicting, such as possessing sufficient strength to survive the casting process, while also being easy to de-core. The granular nature of the material, combined with layered manufacturing, requires a detailed microstructure representation to reproduce these defining characteristics. More precisely, the stiffness differs in the layering direction. Part of the anisotropy may be captured by creating the geometric representation in layers [1]. Additionally, the binder distribution must be accounted for accurately. In detail, the binder is distributed in small drops at discrete locations, in regular patterns that are not equally distributed in all directions, which subsequently increases the anisotropy of the effective material behavior.
In this contribution, we present a concept for the geometric description of the sand-binder microstructures to account for the anisotropic binder distribution. Specifically, we focus on sand cores created via a 3D binder-jetting process, as well as how to capture the anisotropic material behavior. First, we present the generation of layered granular microstructures and the addition of the binder. Then, we introduce an extension of the model that includes an anisotropic binder description, which improves the microstructure representation.

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**Hybrid numerical framework for prototypical scalar linear PDE with rough coefficient**

Balazi, Loïc; Deiml, Matthias; Peterseim, Daniel
*Institute of Mathematics, University of Augsburg, Germany*

10:10

In this work we propose to establish a hybrid numerical framework for a prototypical scalar linear PDE with rough coefficient that integrates classical coarse-scale solvers with quantum subroutines for fine-scale corrections. Inspired by localized orthogonal decomposition (LOD), a computational homogenization method [A. Målqvist and D. Peterseim, "Numerical Homogenization by Localized Orthogonal Decomposition", SIAM (2020)], [R. Altmann, P. Henning, and D. Peterseim, "Numerical homogenization beyond scale separation", Acta Numerica 30 (2021)] and the preliminary work on quantum algorithms for finite elements [M. Deiml and D. Peterseim, "Quantum realization of the finite element method", Mathematics of Computation (2025)], we aim to employ quantum-enhanced local problem solvers to capture fine-scale features efficiently within a multi-scale hierarchy. Indeed, LOD uses well-adapted local basis functions defined on patches of coarse elements. The computation of these local basis functions requires the measurement of local quantities of interest. Consequently, this method fits well with the quantum computing paradigm where only such scalar measurements are possible. Our framework practically overcomes the information bottleneck at the quantum-classical interface and thus fully exploits the quantum advantage. We assess our framework with numerical experiments on simulated quantum hardware.

## S08.02: Composites

Date: March 17, 2026 16:30–18:30
Room: KI, M11.42
Chair(s): Eisenträger, Johanna
Klinge, Sandra

**Multiscale Modeling of Damage in Thermoplastic Fiber Composites for Lightweight Structural Applications**

Liu, Tiansheng (1); Li, Xiangfeng (1); Tabib, Majd (1); Kopic, Nadir (1); Cui, Junhe (2); Valsecchi, Michele (2); Kumar, Sanat (2); Fish, Jacob (2); Pineda, Evan (3); Bednarcyk, Brett (3); Simon, Jaan-Willem (1)
*1: University of Wuppertal, Germany*
*2: Columbia University, USA*
*3: NASA Glenn Research Center, USA*

16:30

The increasing demand for lightweight structures in transportation and related sectors has intensified the use of fiber-reinforced thermoplastic composites, driven by their short processing cycles, high toughness, and recyclability. However, their macroscopic performance is controlled by complex damage-driven softening mechanisms originating in the thermoplastic matrix, which exhibits rate-dependent visco-elastoplastic behavior and large inelastic deformations. Existing modeling approaches remain insufficient to reliably predict failure, particularly because woven thermoplastic fiber-reinforced composite laminates involve multiple interacting mechanisms across scales, and conventional multiscale strategies lose objectivity once softening occurs.

In this contribution, we employ a gradient-enhanced visco-hyperelastic-plastic matrix model within resolved composite microstructures. The gradient extension removes the pathological mesh dependence typically associated with softening, enabling mesh-objective microscale predictions even in the presence of highly localized deformation. However, when such localized responses are transferred into a computational homogenization setting, the resulting effective behavior becomes sensitive to the chosen RVE size—revealing a form of scale dependence that cannot be resolved by gradient regularization alone. To address this limitation, we upscale the microscale response using the failure zone homogenization scheme, which accounts for the finite extent of the failure zone during homogenization and mitigates the size sensitivity of RVE-based predictions.

By combining mesh-objective gradient damage at the microscale with size-objective homogenization at the macroscale, the framework establishes a physically consistent link from matrix-level damage

to effective structural behavior. This directly targets key research gaps identified in current modeling efforts and supports the development of predictive, scalable tools for the analysis of thermoplastic composite components under demanding loading scenarios.

**Homogenization of short fiber reinforced thermoplastics with uncertain input parameters**

Hauschel, Vanessa (1,2); Müller, Jonas (1); Kaiser, Jan-Martin (1); Böhlke, Thomas (2) 17:10
*1: Corporate Sector Research and Advance Engineering, Robert Bosch GmbH, Germany*
*2: Institute of Engineering Mechanics, Karlsruhe Institute of Technology (KIT), Germany*

Short fiber reinforced thermoplastics are used in many industrial applications due to their high specific mechanical properties and cost-efficient processibility in the injection molding process. However, the process induces a complex microstructure which directly affects the anisotropy of the material. Due to the different length scales present in the material, the application of multiscale homogenization techniques is required for the prediction of the effective material properties based on the microstructural descriptors and the constitutive properties at the micro scale [1]. Both, mean-field and full-field methods are commonly applied for this purpose [2,3]. However, the mentioned input parameters are directly affected by material and process variability in a non-deterministic way [4].

Therefore, this contribution focuses on the homogenization of the effective mechanical properties by considering uncertain input parameters. The approach is demonstrated using a short fiber-reinforced polypropylene. The microstructural descriptors such as fiber aspect ratio, fiber volume fraction and fiber orientation tensor were identified using micro-computed tomography. The mechanical properties of the fibers are considered constant, whereas the matrix properties were reverse engineered based on tensile test results. The impact of selected uncertain input parameters on the effective macroscopic material response is evaluated as a basis for probabilistic simulation chain workflows.

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**Evaluating the benefits of the subsampling approach to stochastic homogenization for industrial composites**

Sentler, Tim (1); Schneider, Matti (1,2,3) 17:30
*1: University of Duisburg-Essen, Germany*
*2: Center for Nanointegration Duisburg-Essen (CENIDE)*
*3: Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern*

Computing effective material properties of microstructures using the representative volume element (RVE) method without suitable pre- and postprocessing yields inaccurate results. Notably, non-periodic microstructures, as obtained from real-world samples, lead to errors which are roughly an order of magnitude higher compared to periodized ensembles regardless of the boundary conditions chosen [1-3]. One promising postprocessing strategy recently proven to be effective [4] for simple microstructures is averaging the strain and stress fields on subvolumes only. We numerically investigate the improvement of the magnitude and decay rate of the errors when computing effective material

properties using this subsample averaging. The microstructures investigated are of industrial complexity and scale. We deduce insights for practical engineering use to improve the quality of material properties obtained from available data.

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**Computational homogenization based on adaptive laminates**

Kurzeja, Patrick; Wilbuer, Hendrik; Mosler, Jörn
*Institute of Mechanics, TU Dortmund, Germany*

17:50

Within the context of computational homogenization of mechanical microstructures, adaptive laminates offer a versatile framework for studying how microstructural evolution drives nonlinear and history-dependent effective mechanical behavior [1–3]. For this purpose, the present investigation proposes an adaptive laminate framework and compares it with classic refinement strategies in finite element analyses [4,5]. The key idea is to refine the laminates in a representative volume element (RVE) according to an error-estimator criterion for energy-based relaxation. (Partial) rank-1 homogenization is employed, yielding a rank-1 convex envelope of the initial free energy. Microstructures with different inclusion geometries are tested to assess the performance and robustness of the algorithm in comparison with established refinement strategies. Furthermore, hyperelastic and elastoplastic material behavior are compared using a variational incremental update scheme. Finally, the split frequency, normal vector orientations, and deformation jumps are discussed with respect to their roles within the optimization algorithm.

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**A Temperature-Dependent Mean-Field Modeling Framework Incorporating Damage Evolution for CFRP Machining Processes**

Zhan, Yingjie; Caylak, Ismail; Ostwald, Richard
*Chair of Structural and Materials Mechanics (SWM), University of Paderborn, Paderborn, Germany*

18:10

This work presents a temperature-dependent theoretical and numerical framework for simulating the machining behavior of carbon fiber-reinforced plastics (CFRP). The study first analyzes the limitations of conventional mean-field formulations and introduces an extended four-step mean-field

approach that incorporates micromechanical damage and temperature effects. Constitutive relations for the fiber, matrix, and interface phases are formulated to capture both temperature- and strain-rate-dependent responses. Material parameters are identified from tensile and compression tests on the individual constituents. The resulting temperature-dependent damage-coupled mean-field model is applied to the simulation of CFRP milling, and the simulation results demonstrate a high level of consistency with experimental observations, confirming the predictive capability of the proposed approach.

## S08.03: Homogenization

Date: March 18, 2026 08:30–09:30
Room: KI, M11.42
Chair(s): Simon, Jaan-Willem
von Oertzen, Vincent

### Real-time multiscale exploration of grain boundary effects on diffusion in solid electrolytes

Scholz, Lena; Ou, Yongliang; Keshav, Sanath; Grabowski, Blazej; Fritzen, Felix 08:30
*University of Stuttgart, Germany*

The diffusion behavior of ions in solid-state electrolytes is crucial for the overall performance of solid-state batteries. Studies on the atomistic scale indicate that grain boundary (GB) effects and grain as well as particle size significantly impact overall diffusivity. Recent advances have enabled large-scale, long-time, and high-accuracy simulations of complex atomic structures using ab initio-based machine-learning interatomic potentials [1]. Despite their promising insights, these approaches still go along with massive computational demands, thereby leaving a significant gap between atomistic and application length scales of interest. In simulations on a larger scale, however, the details of the polycrystalline structure are often neglected or only considered under strong assumptions.

We propose a microscopic finite element model [2] that considers the fully resolved crystalline structure with a parametrization that aligns with the atomistic perspective: The potentially anisotropic diffusion coefficients in bulk and GB stem from calculations on atomistic scale and a novel collapsed interface element is introduced to represent GB effects. Furthermore, we account for geometric defects such as pores. By means of homogenization, an effective model on the mesoscale is derived.
The hybrid bulk-interface diffusion model was found to give consistent results when compared with fully-resolved GB representations across the transition from nano- to micrograin regime. Furthermore, we could prove a reasonable agreement with both atomistic bicrystal data and the conductivity measured in experimental setups.
To facilitate an in-depth analysis of material and structural features that govern the effective diffusion behavior, the affine structure of the problem is exploited to derive a reduced-order model. The availability of just a few full simulations enables highly accurate real-time estimates for the effective diffusion coefficients across the parameter space. This enables rapid identification of preferred diffusion paths and a quantitative assessment of how defects, such as GBs or pores, contribute to the overall diffusivity.

Interactive parameter space exploration supports bridging the gap between the concepts on different scales as well as computational and experimental results. This facilitates in silico exploration of microstructures and their implications on larger scales, which enables us to suggest design principles for solid electrolytes with a special focus on GBs.

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**Time Homogenization of Nonlinear Mechanically-Coupled Phase Evolution Based on Low-Pass Convolution**

von Oertzen, Vincent; Kiefer, Bjoern 08:50
*TU Bergakademie Freiberg, Germany*

The modeling of stress-induced phase transformations by means of mechanically-coupled phase-field models typically results in a nonlinear system of partial differential equations. Under cyclic mechanical loading, the local phase state therefore evolves nonlinearly within each load cycle, leading to computationally expensive long-term simulations. This issue is particularly pronounced in case of two- and three-dimensional microstructure evolution, where each cycle must be temporally resolved with sufficient fidelity, see [1]. Although recently proposed cycle jump techniques—typically applied to phase-field fracture models, cf. [2]—offer a potential reduction in computational costs, their accuracy is strongly limited by the number of extrapolated load cycles. This limitation arises because these methods primarily alter the numerical solution procedure, rather than the governing model itself. In contrast, classical homogenization schemes based on asymptotic expansion, such as [3], rely on the existence of temporal scale separation and are mainly designed for linear systems—assumptions that are generally violated in mechanically coupled phase-field models.

To overcome these restrictions, this work introduces a novel homogenization framework that replaces the original nonlinear system with an auxiliary, time-homogenized formulation. The approach is motivated by recently developed spatial homogenization techniques for phase transforming systems, as outlined in [4], and based on a variable low-pass convolution of higher-order modes of the external mechanical loading signal. Most importantly, the existence of temporal scale separation is not required in the proposed framework. Its theoretical foundations are presented for a simplified, yet nonlinear, one-dimensional phase-field model of stress-induced phase transformation. In addition, extensions to higher spatial dimensions are discussed and demonstrated by finite element simulations of cyclic two-dimensional microstructure evolution, incorporating more complex interface topologies.

In summary, the principle advantage of the proposed time homogenization scheme is that the required temporal increment size scales with the selected low-pass frequency, while maintaining constant solution accuracy. As a result, a large number of loading cycles can therefore be simulated significantly faster, without compromising the qualitative trends of the effective phase evolution.

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**Multiscale Simulation of Porous Materials Using FE–FFT Homogenization**

Dahler, Julian (1,2); Scheunemann, Lisa (3); Staub, Sarah (2) 09:10
*1: RPTU Kaiserslautern-Landau, Germany*
*2: Fraunhofer ITWM, Germany*
*3: RWTH Aachen, Germany*

High-performance porous materials with functionally graded microstructures are increasingly used in lightweight and multifunctional applications. Recently, hybrid porous structures with graded layers have come into the focus of research where the macroscopic mechanical response emerges from complex interactions between spatially varying pore architecture, heterogeneous material phases, and multiscale deformation mechanisms. Accurate computational prediction of such materials requires methods that efficiently handle structural-level boundary conditions, gradients in microstructural properties, and strong material heterogeneity at the microscale while accommodating nonlinear constitutive behavior across scales.

This contribution presents a FE-FFT multiscale simulation framework, similar to [1], that couples Finite-Element (FE) methods for macroscopic analysis with FFT-based solvers for microscale homogenization using the open-source coupling library preCICE [2]. The coupling architecture promises modular integration of specialized simulation tools while maintaining numerical efficiency. At the macroscale, a finite strain FE formulation implemented in Ferrite.jl [3] resolves structural boundary conditions and global displacement fields. At each macroscopic integration point, a microscopic representative volume element (RVE) is analyzed using the FFT-based solver FeelMath [4]. The coupling library preCICE facilitates the two-scale data exchange through a parallel communication framework. The partitioned enables efficient load balancing for RVE computations.

We test the developed framework on several numerical examples of porous composites with complex pore architecture.

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## S08.04: Machine Learning and Quantum Computing

Date: March 18, 2026 14:00–16:00
Room: KI, M11.42
Chair(s): Weeger, Oliver
Otto, Alexandra

### X-ray Computed Tomography and Convolutional Neural Network-Driven Multiscale Characterization of Glass Fiber Composites

Bab, Yonca (1,2); Bachhav, Bhagyashri (2); Navrath, Uwe (2); Dorduncu, Mehmet (3); Kutlu, Akif (1); Markert, Bernd (2) 14:00

*1: Department of Civil Engineering, Istanbul Technical University, Istanbul, Türkiye*
*2: Institute of General Mechanics, RWTH Aachen University, Aachen, Germany*
*3: Department of Mechanical Engineering, Izmir Institute of Technology, Izmir, Türkiye*

Accurate prediction of effective in-plane mechanical properties of composite materials requires a robust multiscale link between microstructural features and macroscopic response. In this study, a hybrid multiscale framework integrating X-ray computed tomography (CT) and convolutional neural networks (CNNs) is proposed to estimate the effective in-plane elastic properties of glass fiber composites directly from 2D microstructural images.

Composite systems with distinct reinforcement architectures are considered. High-resolution CT scans are acquired in orthogonal planes (XY, YZ, and XZ), with scanning parameters carefully selected to resolve fiber distribution, matrix regions, and void morphology. The resulting CT slices provide statistically representative 2D microstructural information suitable for multiscale analysis while avoiding the computational cost associated with full 3D reconstructions.

The elastic moduli of the constituent unsaturated polyester and epoxy matrix polymers are independently measured within this study using an MTS testing machine. Poisson's ratios of the matrix materials are evaluated using a synchronized GOM optical camera system, enabling full-field strain measurements and the accurate transverse strain estimation. These experimentally measured matrix properties provide reliable ground-truth inputs for the multiscale modeling framework.

For the data-driven stage, CT slices are decomposed into multiple local patches, each inheriting the same macroscopic material labels. A CNN is trained to extract statistically representative microstructural descriptors capturing key features such as fiber orientation dispersion, phase connectivity, void clustering, and matrix continuity. The CNN outputs mixture properties that are integrated with a rule-of-mixtures approach, ensuring physical consistency while allowing data-driven refinement of classical homogenization assumptions.

The results demonstrate that 2D microstructural information is sufficient for accurate prediction of in-plane elastic behavior across different composite architectures. The proposed multiscale CT-CNN framework offers a physically grounded and computationally efficient approach for bridging microstructural statistics and macroscopic mechanical response in glass fiber composites.

**Data-driven Inverse Design and Surrogate Modeling of Spinodoid Architected Materials**

Otto, Alexandra (1); Fritzen, Felix (2); Keshav, Sanath (2); Kalina, Karl Alexander (1); Kästner, Markus (1)

*1: Dresden University of Technology, Chair of Computational and Experimental Solid Mechanics, Germany*
*2: University of Stuttgart, Institute of Applied Mechanics, Data Analytics in Engineering, Germany*

14:20

Mechanical metamaterials enable the tailoring of their macroscopic mechanical response through the careful design of their mesostructural geometry in combination with a given base material. This makes them ideal candidates for inverse design, i.e., the identification of a specific metamaterial with specific mechanical properties [1]. Data-driven inverse design approaches offer an efficient way to explore and invert the resulting high-dimensional design spaces, particularly for architected materials with complex, nonperiodic topologies

In this contribution, we present a neural network-based approach for the inverse design of elastic properties of architected materials, with a focus on spinodoid metamaterials [2]. Spinodoids are characterized by a low-dimensional set of topological descriptors while exhibiting a broad range of anisotropic effective elastic responses.

Beyond linear elasticity, we present initial results on data-driven approximation of the yield surface of spinodoid metamaterials. A kernel-based regression framework is employed to construct a surrogate representation of the initial yield surface from discrete stress-strain data obtained by numerical simulations [3], leveraging concentric interpolation to describe the yield surface in stress space [4]. The presented results are intended to assess the suitability of such surrogate models for capturing the onset of plasticity in architected materials, as well as their potential applicability within inverse design workflows.

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**A Mesh-Based Shallow Energy Method (M-SEM) for highly accurate and robust simulation of heterogeneous composites**

Wichmann, Pius J.M.; Hildebrand, Stefan; Klinge, Sandra

*Technische Universität Berlin, Germany*

14:40

Heterogeneous composites are ubiquitous in engineering and nature, ranging from biological tissues to fiber-reinforced industrial structures. The simulation of these materials is numerically challenging due to discontinuities and stress concentrations caused by substantial contrasts in stiffness. The deep energy method (DEM) has emerged as a versatile physics-informed framework for nonlinear

elastostatics. Variants, such as the shallow energy method (SEM), further improve parallelizability and efficiency. Compared to the finite element method (FEM), the DEM and SEM eliminate the need for second-order derivatives of the system's total potential energy, compiled into a stiffness matrix. Instead, the system's total potential energy is explicitly calculated and included in the loss function for minimization. Despite the highly accurate results for homogeneous bodies, both the DEM and SEM exhibit significant inaccuracies near discontinuities and do not support the simulation of heterogeneous bodies without extensions. To address these issues, a mesh-based shallow energy method (M-SEM) is proposed that combines the flexibility of physics-informed learning with the robustness of finite element discretization and the efficiency of radial basis function neural networks (RBFNNs).

The M-SEM replaces the collocation points used in the SEM with a mesh-based discretization. The use of elements with shape functions and Gaussian quadrature enhances the robustness by eliminating erroneous reductions of the loss value by unphysical spatial oscillations in the displacement output akin to overfitting. The single-layer, fixed-center RBFNN greatly simplifies the loss landscape compared to deep architectures and allows for maximal parallelizability of the computation.

The case studies involve composite materials with ratios of stiffnesses up to 1:1000, hyperelastic materials, and multiple hard inclusions. As a benchmark, the mesh-based formulation is compared with the collocation-based DEM, an extended DEM that employs random Fourier features (RFF), the SEM, as well as a new implementation with a Kolmogorov-Arnold network (KAN). The mesh-based framework reduces errors by up to three orders of magnitude compared to the DEM. One order of magnitude of this reduction is accounted for by the RBFNN architecture instead of a standard multilayer perceptron. Furthermore, the M-SEM reduces the computational effort by one order of magnitude compared to the benchmarks. Consequently, the M-SEM represents a highly efficient, accurate, and robust solver for complex heterogeneous problems in solid mechanics.

**Surrogate elements for nonlinear microstructures using physics-augmented machine learning**

Li, Wei; Weeger, Oliver
*TU Darmstadt, Germany*

15:00

For microstructure materials with non-periodic cells or non-separated scales, such as additively manufactured lattices and metamaterials, multiscale modeling approaches are inapplicable, but full-scale simulations are still prohibitively time-consuming, in particular for nonlinear materials and large deformations. For a fast and efficient nonlinear simulation of such structures, we introduce the concept of surrogate elements, which capture the effective mechanical behaviour of the unit cells of the microstructure only through the boundary nodes. We consider an internal energy potential, which enables the determination of the energy and forces associated with a given deformation of the microstructure's boundary nodes. This potential is represented by a physics-augmented feed-forward neural network that incorporates energy conservation, invariance to rigid body translations and rotations, and normalization conditions. The equilibrium configuration of a macro-structure consisting of many interconnected unit cells is then obtained by minimizing the total potential energy, which is assembled from the microstructure potentials. Here, this concept is demonstrated in application to 2-D beam lattice microstructures. First, a data set for the surrogate potential, forces, and moments is built by performing nonlinear simulations of lattice unit cells subject to different deformation and load cases. Then, a physics-augmented neural network surrogate is trained on this data in order to approximate the functional relationship for the energy potential. We aim to demonstrate the accuracy, efficiency and robustness of the approach through several verification examples, in which these surrogate potentials are applied for the nonlinear simulation of macro-structures.

**A Deep Learning-Enhanced Continuum Micromechanics Framework for Nonlinear Homogenization of Composites with Nonellipsoidal Inclusions Geometries**

Schwaighofer, Michael; Königsberger, Markus; Lukacevic, Markus; Füssl, Josef 15:20
*Institute of Mechanics of Materials and Structures,TU Wien, Austria*

The macroscopic mechanical response of heterogeneous materials is dictated by the morphology and mechanical properties of their constituents. While classical mean-field homogenization schemes based on Eshelby-type solutions [1] are computationally efficient, they typically rely on idealized inclusion geometries and uniform strain assumptions, which limit their accuracy in nonlinear regimes. Full-field computational homogenization overcomes these restrictions but remains computationally expensive. Recent data-driven approaches [2] offer a potential alternative for nonlinear materials, yet their applicability is often hindered by limited generalizability across different microstructures and the requirement for explicit microstructure generation.

This work proposes a hybrid micromechanical framework that integrates finite element-based Eshelby analysis with continuum micromechanics and machine learning to enable the efficient nonlinear homogenization of composites with plastic material behavior. The core innovation involves replacing the single, average strain concentration tensor of analytical solutions with a discretized strain concentration field extracted from finite element simulations of Eshelby problems with non-ellipsoidal, superspherical inclusions. By capturing these local strain heterogeneities, the framework enables the progressive plasticization of material phases within continuum micromechanics theories, resulting in a more physically representative macroscopic response.

The methodology begins by numerically solving the Eshelby problem for superspherical geometries across a wide range of phase stiffness contrasts. The resulting strain concentration tensors are clustered into groups based on their similar mechanical responses, and a neural network is trained to predict these clustered tensors as a function of inclusion geometry and phase properties. The network is then integrated into a continuum micromechanics scheme by treating each cluster as an individual phase. By considering plastic strains as eigenstrains within these clusters and upscaling them, the macroscopic nonlinear behavior is computed. Predicted stress-strain responses for composites exhibiting Von Mises plasticity and isotropic hardening agree well with full-field simulations. Ultimately, the proposed framework provides an efficient and robust means of homogenizing composites with non-ellipsoidal inclusions and nonlinear material behavior without the need for explicit microstructure generation.

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**A software framework for model adaptivity in mechanical multiscale coupled problems**

Hocks, Alex (1); Desai, Ishaan (2); Uekermann, Benjamin (2) 15:40
*1: Technical University of Munich, Germany*
*2: University of Stuttgart*

In mechanical system models involving advanced materials, a multiscale treatment is required. However, solving micro-scale problems is often computationally expensive. Therefore, adaptive strategies are necessary. The aim of this work is to implement new functionality in existing coupling software to facilitate the coupling of two or more scales with model adaptivity, with a particular focus on mechanical system modeling. The software stack consists of the coupling library preCICE and the so-called Micro Manager - a Python-based tool that initializes and controls a large number of micro-scale simulations and communicates with preCICE.

Currently, the Micro Manager employs the adaptivity strategy proposed by Bastidas et al., which partitions micro-scale simulations into active and inactive sets. The active simulations are solved explicitly, and their results are transferred to the most similar inactive simulations. In this work, a more elaborate model-based adaptive strategy for mechanical system modeling, proposed by Fritzen, is implemented. This strategy relies on a hierarchy of models that are dynamically switched based on model-specific parameters. The hierarchy ranges from full-order models (FOMs) to reduced-order models (ROMs), and further includes artificial neural networks (ANNs).
The implemented functionality is verified and benchmarked in a setup where preCICE couples the Micro Manager - utilizing the FFT-based micromechanics solver FANS - to a mesoscopic mechanics solver. The latter is a finite element method (FEM) code based on FEniCSx, supporting both small- and large-strain formulations. First, the mesoscopic solver is verified, including mesh refinement studies. Subsequently, the benchmark setup is evaluated for different scenarios using FANS as the FOM. The ROM, based on a singular value decomposition (SVD) approach, and the ANN, a data-driven model with physical guarantees, are provided by domain experts Fritzen et al. The results demonstrate that a significant reduction in computational time can be achieved, provided that the ROM and ANN are reusable.

## S08.05: Porous Media and Interfaces

Date: March 18, 2026 16:30–18:30
Room: KI, M11.42
Chair(s): Kurzeja, Patrick
Klinge, Sandra

### Numerical Homogenization of Different Foam Materials using FFT-based Methods

Staub, Sarah (1,2); Andrä, Heiko (1); Dahler, Julian (1,3) 16:30
*1: Fraunhofer ITWM*
*2: DHBW Mannheim*
*3: RPTU Kaiserslautern-Landau*

Foam materials play a crucial role across engineering sectors, including polyurethane (PU) foams for automotive seating and household insulation, and aluminum foams for lightweight structures and crash absorption. The macroscopic behavior of these foams strongly depends on their bulk material as well as on the microstructure. Particularly the cell topology and connectivity, which distinguish open-cell from closed-cell foams and may include partially closed cells, e.g., in dense PU systems.

In this work we focus on the computation of different foam systems. Based on the foaming simulation of a car seat, which results in inhomogeneous PU densities at different locations, microstructures with low, medium and high solid volume fractions are generated. The effective material behavior of the different structures is computed and compared to experimental data. Due to the properties of the PU, these foams behave nonlinear elastic even at high strains, up to 70% compression.

As a second class of foams, aluminum (Al) foams are considered. A special application concerns so-called hybrid porous media which are investigated within the DFG TRR375 Hypo project [1]. Thereby, weight-optimized parts comprising a porous Al-foam core reinforced by an added nonporous outer layer are addressed. Due to the elastoplastic behavior of the aluminum and the applied additive manufacturing process thermally induced residual stresses arise, which influence the effective foam behavior. In a first step the elastoplastic behavior of Al foams is computed and compared to macroscopic models, such as the Deshpande-Fleck [2] model. In a second step the influence of heat onto the effective behavior is studied.

In this work, we apply FFT-based solvers for the periodic boundary value problem in elasticity for RVEs to perform numerical homogenization of diverse foam microstructures [3]. Therefore, ITWM's solver FeelMath is used for simulations [4]. The modelling of the specific bulk materials (PU and Al), the microstructure generation based on SEM and CT images are discussed.

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[3] Liebscher, A., Andrä, H., Kabel, M., Merkert, D., and Redenbach, C. "Modelling open cell foams based on 3D image data." In *Proceedings of the 20th International Conference on Composite Materials*, 2-5, 2015.

[4] Fraunhofer ITWM: FeelMath, https://www.itwm.fraunhofer.de/feelmath, accessed: 08.01.2026

**Asymptotic Reduction Modeling for Partially Saturated Soil Based on the Theory of Porous Media**

Araz, Firat; Seyedpour, Seyed Morteza; Ricken, Tim; Armiti-Juber, Alaa 17:10
*ISD, Universittät Stuttgart, Germany*

The comprehensive depiction of fluid saturated soil mechanics necessitates the integration of field equations from solid and fluid continuum mechanics in a coupled manner. This integration yields a cohesive set of equations capable of elucidating prominent phenomena like fluid flow through a porous deforming solid matrix not merely in isolation but as interrelated and interacting complexities. Consequently, this approach aligns closely with the complex behavior observed in real fluid saturated soils. However, describing a single fluid occupying the pore space, despite accounting for multi phase mechanics, the absence of a second fluid phase in the common models renders the application of mechanical stress and strain without the introduction of capillary pressure. Thus, they fail to capture the intricate mechanical behaviors between a liquid and a gaseous phase in porous materials subjected to substantial solid deformation and their inherent impact on filtration processes.

The modeling of multi-phase materials can be done by employing the Theory of Porous Media (TPM). TPM is very effective for saturated soil modeling due to its capacity to describe multi-phase and multi-component domains. This approach enables simultaneous representation of solid and fluid materials, utilizing homogenized fields. It allows for the depiction of porous solid matrix deformation under thermal and mechanical influences while capturing fluid motion, specifically within the Darcy regime for velocity fields. Consequently, it facilitates modeling the transport mechanisms between a mobile gas and a liquid as individual constituents of the fluid body, driven by pressure gradients and capillary effects.

The coupled field equations are defined within a thin rectangular computation domain, possessing an aspect ratio conducive to employing the model order reduction technique of asymptotic analysis. This approach facilitates dimensional reduction within the computation domain. Consequently, two sets of field equations combine to substitute the high-fidelity model. The first, a dimensionally reduced limited model, describes deformation in the large-scale direction, while the second, the corrector model, reinstates effects in the small-scale direction.

**A second-order multi-scale phase-field fracture model for hydro-mechanically coupled porous materials**

Polukhov, Elten; Marulkar, Vedant; Keip, Marc-André 17:30
*University of Stuttgart, Germany*

Porous materials are commonly described as coupled systems consisting of a porous solid skeleton and a fluid phase, in which fluid transport strongly influences the mechanical response and deformation of the material. Such hydro-mechanical coupling is observed in geomaterials, biological systems, battery components, and some implant materials. While these interactions are essential to many applications, they can also lead to material failure. In hydraulic fracking, fractures are intentionally induced to enhance permeability in geomaterials, whereas in battery components and implant materials it may result in premature degradation and reduced service life. In addition, understanding the environmental implications of hydraulic fracturing, including the potential contamination of groundwater resources, are important to investigate.

In this contribution, we investigate hydro-mechanically induced fracturing in heterogeneous porous structures using a second-order two-scale modeling framework [1, 2]. The approach couples a Darcy–Biot model at the microscale with a gradient-enhanced poromechanics model at the macroscale. By incorporating second-order gradients of the macroscopic primary fields, the framework enriches the microscale problem with higher-order deformation and flow modes and relaxes the classical scale separation assumption [3, 4, 5]. This enables the modeling of hydraulic fracturing, softening behavior, and intrinsic length-scale effects. The presentation outlines the modeling framework and its numerical implementation, followed by numerical examples illustrating fluid-driven fracture initiation and propagation in elastic porous structures.

**References**

[1] E. Polukhov and M.-A. Keip. Second-Order Computational Homogenization of Nonlinear Fluid Flow through Porous Media. *International Journal for Numerical Methods in Engineering*, 127:e70100, (2026).
[2] Miehe, Christian, Steffen Mauthe, and Stephan Teichtmeister. Minimization principles for the coupled problem of Darcy-Biot-type fluid transport in porous media linked to phase field modeling of fracture. *Journal of the Mechanics and Physics of Solids*, 82, 186–217 (2015).
[3] V.G. Kouznetsova, M.G.D. Geers and W.A.M. Brekelmans. Multi-scale second-order computational homogenization of multi-phase materials: a nested finite element solution strategy. *Computer methods in Applied Mechanics and Engineering*, 193, 5525–5550 (2020).
[4] I. A. Rodrigues Lopez, and F. M. Andrade Pires. Unlocking the potential of second-order computational homogenisation: An overview of distinct formulations and a guide for their implementation.*Archives of Computational Methods in Engineering*, 1–55 (2021).
[5] E. Polukhov and M.-A. Keip. Computational homogenization of transient chemo-mechanical processes based on a variational minimization principle. *Advanced Modeling and Simulation in Engineering Sciences*, 7, 1–26 (2020).

**A Top-Down Thermodynamic Motivated Perspective on Multiscale Material Modeling**

Warkentin, Andreas; Ricoeur, Andreas 17:50
*Universität Kassel, Institute of Mechanics, Engineering Mechanics/ Continuum Mechanics, Germany*

Multiscale models, usually bottom-up approaches, are indispensable in the numerical modeling of complex materials. Their computational efficiency relies on model reduction strategies whose underlying assumptions regarding homogenization, however, often remain implicit and therefore only limitedly controllable. The following approach attempts to provide a preliminary answer to this question.

In this contribution, a thermodynamic recursive multiscale framework is introduced, which formulates multiscale modeling consistently as a top-down problem [1]. The starting point is a simple yet strict requirement: for each system, the first law of thermodynamics holds locally, while the internal energetic state (internal energy) of a system is determined by a recursive aggregation of the total energies of the next smaller scale.

For illustration, the framework can be interpreted as a tree structure in the sense of computer science. Each node represents a system defined on a specific scale; nodes on lower levels determine, in an energetic sense, the state of higher levels without losing their system identity. The tree representation does not describe a geometric decomposition but rather a precise mapping structure for scale coupling.

On this basis, established multiscale approaches, e.g., the condensed method [2,3,4] and $FE^2$ formulations, can be understood as special cases of this framework. It is shown that the reduction of numerical degrees of freedom observed in these approaches follows directly from the underlying assumptions. This approach renders these assumptions explicit and allows for their systematic analysis and variation.

Furthermore, the incorporation of existing constitutive potentials within this framework merits particular attention, as such potentials are valid exactly on the scale for which they are formulated. A further

resolution toward smaller scales is possible, provided that the aggregation of subscale contributions reproduces the potential defined on the higher scale upon upscaling.

[1] A. Warkentin, Entropy, 27(9), 976 (2025).

[2] S. Lange, A. Ricoeur, Int. J. Solid Struct., 54, 100-110, (2015)

[3] A. Warkentin, L. Behlen and A. Ricoeur, Smart Mater. Struct. 10.1088/1361-665X/acafba (2023).

[4] L. Behlen, A. Warkentin and A. Ricoeur, Smart Mater. Struct. 30, 035031 (2021).

**A multiscale view on grain boundary resistivity and the Andrews method**

Kaiser, Tobias (1); Güzel, Dilek (1); Bishara, Hanna (2); Dehm, Gerhard (3); Menzel, Andreas (1,4)

*1: Institute of Mechanics, TU Dortmund University, Germany*
*2: Department of Materials Science and Engineering, Tel Aviv University, Israel*
*3: Max Planck Institute for Sustainable Materials, Germany*
*4: Division of Solid Mechanics, Lund University, Sweden*

18:10

In this work, we focus on microscale material interfaces in the form of grain boundaries and study their effect on the effective properties of electrical conductors.

To this end, we make use of classic energy-based computational multiscale approaches for bulk materials and extend these to resistive material interfaces [1]. In particular, we derive an extended set of scale-bridging relations that explicitly accounts for the presence of cohesive-type material interfaces at the microscale and show energetic consistency of both scales in the sense of Hill-Mandel. We embed the extended multiscale formulation for electrical conductors into a finite-element-based multiscale code and study elementary academic boundary value problems. In doing so, we demonstrate the usefulness of the proposed approach to extract effective conductivity tensors for complex microstructures and show the importance of the intrinsic length scale induced by the presence of microscale interfaces.

In a second step, we revisit the Andrews method that has been a focal point of discussion in the materials science community since the late 1960s and that is used to predict the effective resistivity of polycrystals by accounting for the single crystal resistivity, the average grain boundary resistivity, and grain geometry factors. We show that this purely phenomenological approach is under certain restrictive conditions consistent with computational multiscale schemes, discuss the importance of (quasi-)isotropy, resolve its core limitations and eventually validate the simulation-based predictions against experimental data [2].

[1] Güzel D., Kaiser T., Menzel A., A computational multiscale approach towards the modelling of microstructures with material interfaces in electrical conductors. Mathematics and Mechanics of Solids, Vol. 30 (2), 247–266, 2025, doi: 10.1177/10812865231202721.

[2] Güzel D., Kaiser T., Bishara H., Dehm G., Menzel A., Revisiting Andrews method and grain boundary resistivity from a computational multiscale perspective. Mechanics of Materials, Vol. 198 (1), 105115, 2024, doi: 10.1016/j.mechmat.2024.105115.

**S08.06: Model Reduction and FE2**

Date: March 19, 2026 08:30–10:30
Room: KI, M11.42
Chair(s): Wulfinghoff, Stephan
Staub, Sarah

**Graph-based nonlinear model order reduction for computations on representative volume elements**

Faust, Erik; Scheunemann, Lisa 08:30
*Institute of Applied Mechanics, RWTH Aachen University, Germany*

Coupled multiscale simulations using the FE² method require microscopic simulations on representative volume elements (RVEs) with thousands of different macroscopic deformation gradient values attached to each macroscopic Gauss point. In such a parameterised multi-query context, projection-based model order reduction methods can reduce online runtime by multiple orders of magnitude without significantly compromising accuracy [1].

In particular, projection-based model reduction techniques working with nonlinear approximation spaces can yield accurate reduced order models with a dimensionality that is close to that of the solution manifold. We proposed one such projection-based model reduction scheme using graph-based manifold learning techniques in [1]. If the low-dimensional reduced models constructed this way also facilitate the construction of accurate low-order hyperreduction models, this enables further reductions in runtime, while accuracy is maintained [2].

In this work, we explore the performance of several nonlinear projection-based model order reduction schemes on an example quasi-static RVE problem. We also investigate several popular hyperreduction techniques as well as recent developments, and explore the performance achived in terms of runtime and accuracy for a range of model parameters.

[1] Scheunemann, L., Faust, E. A manifold learning approach to nonlinear model order reduction of quasi-static problems in solid mechanics: proof of concept and parameter study. Comput Mech (2025). https://doi.org/10.1007/s00466-025-02696-0

[2] Faust, Erik, and Lisa Scheunemann. "A hyperreduced manifold learning approach to nonlinear model order reduction for the homogenisation of hyperelastic RVEs." arXiv preprint arXiv:2508.21527 (2025).

**E3C: A Novel Hyper-Reduction Technique For Two-Scale Modeling Applied To Elastoplasticity**

Goldbeck, Hauke; Wulfinghoff, Stephan 08:50
*CAU Kiel, Germany*

We present a recently developed hyper-reduction technique called Empirically Corrected Cluster Cubature (E3C) and its application to two-scale elastoplasticity. The method identifies a reduced set of integration points trough preliminary clustering and empirically corrects them trough a cost function minimization. The approach is applied to a computationally homogenized elastoplastic material model.

**Efficient Computational Homogenization of Dissipative Microstructures using an Empirically Corrected Cluster Cubature Hyper-Reduction Method**

Wulfinghoff, Stephan; Hauck, Jan; Goldbeck, Hauke 09:10
*Kiel University, Germany*

Computational homogenization methods open the possibility to simulate engineering structures on two scales simultaneously and to accurately describe complex macroscopic material behavior. Their intrinsically high computational cost can be alleviated through model order reduction methods in combination with hyper-reduction. The recently proposed E3C hyper-reduction method is applied to various computational homogenization problems, including hyperelasticity, von Mises plasticity, crystal plasticity and magnetism with hysteresis. It is found that errors in the order of 1% are obtained for small numbers of integration points, often in the order of 10-30, depending on the application.

**A multiscale model reduction framework for nonlinear solder joint reliability analysis**

Feuchter, Mike (1); Baumgartl, Hanna (1); Hanke, Martin (1); Rzepka, Sven (2) 09:30
*1: CADFEM Germany GmbH*
*2: Fraunhofer ENAS*

Automotive electronic control units (ECUs) increasingly rely on chiplet-based architectures, in which multiple computing dies are assembled on a single substrate to increase computational performance while limiting manufacturing cost. While the overall number of solder joints does not increase compared to monolithic solutions, chiplet-based layouts significantly alter the internal load distribution. Highly stressed solder joints are therefore no longer confined to well-defined locations such as package corners, which prevents the use of locally refined meshes and leads to substantially larger finite-element (FE) models.

Under thermomechanical loading, solder joints exhibit rate-dependent viscoplastic behaviour, and the accumulated plastic work per thermal cycle is widely used as an indicator for damage evolution and reliability assessment. Accurate prediction of this quantity requires high-fidelity FE simulations; however, the resulting large-scale nonlinear models—often comprising several million elements ( 3.5 million in this study)—are computationally expensive and restrict their use in reliability-driven design studies.

This contribution introduces **HYPER-SUB (HYbrid Parametric and Energy-based Reduction for SUBstructuring)**, a scalable **model reduction framework** tailored to solder joint reliability analysis. Within a single substructure, local nonlinear solder joint behaviour is embedded into the global structural response by combining linear, temperature-dependent components (e.g. copper pads) with nonlinear components governed by viscoplastic solder behaviour described by the Anand material model. The nonlinear solder balls are reduced using an **energy-conserving sampling and weighting (ECSW)** hyperreduction technique to preserve the contribution of internal work terms. A physically motivated error estimator based on the accumulated plastic work is employed to adaptively select both the number of reduced modes and sampled elements.

The approach is applied to an automotive thermal cycling profile consisting of an initialization at 180 °C followed by two cycles between -40 °C and 125 °C. The reduced model predicts the accumulated plastic work per cycle and per solder ball with errors of approximately 10 % relative to the full-order FE solution. Although the reduction is applied exclusively to the solder balls—representing roughly 30 % of the total element count—a computational speedup of about a factor of 2 is achieved. The framework is fully implemented within a commercial FE environment (ANSYS), can be seamlessly coupled to unreduced full-order FE components within the same solver workflow, and is transferable to other nonlinear material models beyond viscoplastic solder joints.

**Multiscale modelling of frame structures with lattice-like microstructures using finite beam elements at the macro and micro levels**

Ochs, Julian; Wackerfuß, Jens 09:50
*University of Kassel, Germany*

Lattice materials are characterized by a high stiffness-to-mass ratio and offer significant potential for engineering applications. This contribution investigates their use in the context of frame structures, focusing on microstructures with a periodic arrangement of identical cells. The geometric complexity of lattice structures has long posed a challenge for manufacturing; however, advances in additive manufacturing now enable the efficient and precise production of highly complex microstructures. As a result, the numerical description of their mechanical behaviour has gained increasing importance. One approach is the direct simulation of the entire structure, which allows for detailed analysis but entails considerable computational cost. Among the efficient alternatives provided by hierarchical multiscale models, an $FE^2$-based model is considered here.

In the $FE^2$ method, two finite element analyses on the macro- and microscale are coupled. In the classical $FE^2$ approach, both scales are modelled continuously, for which numerous formulations exist (e.g., Miehe and Koch [5]). Approaches have also been proposed for continuous macrostructures

combined with lattice-like microstructures (e.g., Danesh et al. [1]). By contrast, the use of structural models at the macroscale with a continuous microstructure is a relatively recent development (e.g., Geers et al. [2], Gruttmann and Wagner [3], Klarmann et al. [4]). A key feature of this approach is the special treatment of the representative volume element (RVE), where a distinction is made between a physical and a model boundary. A major challenge is ensuring that the homogenised material parameters remain independent of the RVE length, which can be achieved through the introduction of appropriate constraints.

The present work adopts this modelling concept and extends it to lattice-like microstructures. The development of the representative volume element from the underlying microstructure is presented, with the RVE being modelled using finite beam elements. Furthermore, the adaptation of constraints originally formulated for continuous microstructures to lattice-like microstructures is presented. Finally, the performance of the proposed FE² model is demonstrated using selected numerical examples, with comparisons to direct numerical simulations.

[1] Danesh et al., *Results in Engineering*, 25, 103976 (2025).
[2] Geers et al., *Modell. Simul. Mater. Sci. Eng.*, 15(4), S393 (2007).
[3] Gruttmann & Wagner, *Int. J. Numer. Methods Eng.*, 94, 1233–1254 (2013).
[4] Klarmann et al., *Computational Mechanics*, 65, 635–661 (2020).
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**A Multi-scale Phase Field Framework for FE²**

Hütter, Geralf; Lathiya, Fenil Maganbhai; von Oertzen, Vincent; Kiefer, Bjoern 10:10
*TU Bergakademie Freiberg, Germany*

Phase-field modeling has become a key tool for describing microstructure evolution in materials. However, classical simulations are typically limited to small representative samples due to their high computational cost and lack of direct connection to structural-scale fields. In this contribution, a **phase-field homogenization framework** is presented that embeds microscopic phase-field models within a macroscopic continuum formulation using a **two-scale finite element (FE²) approach**.

The method establishes a consistent energetic coupling between microscopic phase evolution and macroscopic deformation. The local microstructure, represented by an evolving order parameter, is resolved on the microscale and its effect on the global response is captured through computational homogenization. This enables simulation of complex phase transformation processes in entire components, while still accounting for the underlying microstructural kinetics.

First numerical results demonstrate the feasibility of the approach and highlight its potential for predictive, structure-scale modeling of materials with evolving microstructures. The framework opens the door for multi-scale analysis of transformation, damage, and patterning phenomena in realistic geometries—linking microstructural physics with component-level mechanics within a unified continuum setting.

## S08.07: Advanced Constitutive and Structural Behaviour

Date: March 19, 2026 14:00–16:00
Room: KI, M11.42
Chair(s): Blaszczyk, Mischa
Hütter, Geralf

**Stochastic description of the mechanical response in network glasses**

Wu, Zhao (1); Bamer, Franz (1); Simon, Jaan-Willem (2); Markert, Bernd (1) 14:00
*1: RWTH Aachen, Germany*
*2: Bergische Universität Wuppertal*

Understanding damage and fracture in disordered network materials remains a fundamental challenge [1]. Material failure is a multiscale problem originating from elementary events on the nanoscale whose identification requires numerically expensive molecular simulations. In this contribution, we

generate an entire set of fracture simulations using molecular mechanical descriptions under athermal quasi-static conditions. We develop a data-driven stepping scheme that considers mechanically driven elementary events in a probabilistic sense. The model can describe the evolution of plastic deformation and fracture with insignificant computational effort, offering an attractive tool that can be incorporated into a multiscale modeling framework.

[1] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng., (2023), https://doi.org/10.1007/s11831-022-09861-1.

**Computational Relaxation Techniques for Isotropic Functions**

Balzani, Daniel (1); Köhler, Maximilian (1); Neumeier, Timo (2); Peter, Malte A. (2); Peterseim, Daniel (2); Wiedemann, David (3)

*1: Ruhr University Bochum, Germany*
*2: University of Augsburg, Germany*
*3: TU Dortmund University, Germany*

14:20

The numerical approximation of nonlinear variational models in continuum mechanics with non-convex energy densities, such as those arising in finite strain damage and phase transition models, often suffers from mesh sensitivity and numerical instabilities. Relaxation by means of semi-convexification provides a consistent variational framework to address these issues, guaranteeing the existence of minimisers and yielding mesh-independent approximations. In addition, the relaxation process exhibits a multiscale character and allows for the identification of emerging microstructures, such as laminates.

This talk addresses computational semi-convexification techniques for isotropic energy densities. For the approximation of the polyconvex envelope, the signed singular value characterisation of isotropic functions is employed to reduce the convexification problem from the lifted d×d deformation-gradient space to a d-dimensional manifold in the minors-lifted space. This dimension reduction, combined with established optimisation and computational geometry algorithms, leads to a substantial reduction in computational complexity.

In addition, an approach for the efficient approximation of the rank-one convex envelope of isotropic functions is presented. The method exploits the dimension-reduced characterisation and the associated symmetries of isotropic functions via signed singular values for an accelerated computation, simultaneously providing a direct microstructural description of laminates in the signed singular value space. A series of numerical experiments demonstrates a substantial computational speed-up compared to existing algorithmic approaches, along with enhanced stability, thus paving the way for concurrent relaxation in simulations of boundary value problems.

**Adaptive grid refinement in FFT-based homogenisation by using interpolatory wavelets**

Mätzig, Laurenz (1); Kaiser, Tobias (1); Raasch, Thorsten (2); Remmers, Joris J. C. (3); Geers, Marc G. D. (3); Menzel, Andreas (1,4)

*1: Institute of Mechanics, TU Dortmund University, Germany*
*2: Department of Mathematics, University of Siegen, Germany*
*3: Mechanics of Materials Group, Eindhoven University of Technology, The Netherlands*
*4: Division of Solid Mechanics, Lund University, Sweden*

14:40

In multiscale material modelling, FFT-based methods enable the computationally efficient solution of cell problems. The related solution schemes exploit the fast Fourier transform to evaluate the action of the solution operator on the stress field in the discrete frequency domain at the expense of apointwise tensor contraction. Using the FFT necessitates an equispaced discretisation for the unit cell, which leads to substantial computational effort when modelling materials with localized microscale features and complex constitutive behaviour. In particular, computationally expensive material models must be evaluated on the fine grid across the entire unit cell, including areas where fewer evaluations would suffice to accurately represent the solution field.

Following Kaiser et al. [1], we investigate a strategy that identifies a sparse subset of spatial positions at which the material model is evaluated, while still providing an approximation of the full-grid material response with prescribed accuracy. The proposed adaptive refinement scheme relies on representing the solution fields in a wavelet basis generated by symmetric iterative interpolation processes as described in [2]. By exploiting the multiscale properties of the wavelet transform, the method computes a full-field approximation of the stress response.

In this contribution, we combine the wavelet approach with a staggered grid discretisation [3] so as to significantly improve its stability and accuracy. Compared with the standard wavelet discretisation, the results indicate a substantial reduction in both the number of material model evaluations and the local approximation error. In addition, we extend the analysis of the adaptive refinement scheme to three dimensions and examine its properties in large-scale simulations of polycrystalline materials.

References:
[1] T. Kaiser, T. Raasch, J.J.C. Remmers and M.G.D. Geers: A wavelet-enhanced adaptive hierarchical FFT-based approach for the efficient solution of microscale boundary value problems, Computer Methods in Applied Mechanics and Engineering, 409, 115959, 2023, doi: 10.1016/j.cma.2023.115959.
[2] G. Deslauriers and S. Dubuc: Symmetric iterative interpolation processes, Constructive Approximation, 5, 49–68, 1989, doi: 10.1007/BF01889598.
[3] M. Schneider, F. Ospald, M. Kabel: Computational homogenization of elasticity on a staggered grid, International Journal for Numerical Methods in Engineering, 105, 693–720, 2015, doi: 10.1002/nme.5008.

**On some aspects of scale-dependent multi-continuum homogenization**

Nika, Grigor (1); Veluvali, Shyam (2)
*1: Karlstad University, Sweden*
*2: University of Groningen, the Netherlands*

15:00

Classical homogenization is insufficient for finite-sized structures as it does not account for crucial scale-size effects. We will present a thermodynamically consistent model and subsequent two-scale expansion homogenization framework for strain-gradient elasticity that derives effective models with scale-dependent homogenized coefficients. Our key result is that the homogenized mechanical properties depend not only on the micro-geometry and volume fraction but also on the absolute size of the underlying constituents. Hence, the homogenized coefficients are not constant (as in classical homogenization) but rather functions of the microstructural size.

Numerical validation confirms that the homogenized coefficients converge to the classical ones as the scale-size effects become vanishingly small, providing a critical tool for designing micro-architected materials.

**Computational modeling of the homogenized hydraulic and chemical conductivity in fractured Engineered Cementitious Composites during Self-healing**

Blaszczyk, Mischa; Buegger, Urs; Tofeti-Lima, Thamara; Jänicke, Ralf
*TU Braunschweig, Germany*

15:20

Engineered Cementitious Composites (ECCs) are a class of construction materials reinforced with short fibers possessing remarkable properties. These include ductile material behavior, strain hardening and the ability to self-heal fractures. The latter is enabled by adding significant amounts of unreacted binder within the cementitious matrix. The self-healing process is initiated when ECCs are exposed to water, causing hydration of the matrix and thus sealing fractures over time [1]. For this reason, a possible application of ECCs is the usage as a protective layer to repair existing structures. By limiting crack width under strain, the penetration of water and chloride ions – responsible for corrosion of the embedded steel – is reduced [2].

We investigate the self-healing process by analyzing µ-XRCT (micro X-Ray Computed Tomography) scans of fractures in real ECC samples [3]. The change in morphology is obtained accurately by performing repeated scans over time after water exposure. The scans then serve as input data for numerical simulations. We perform a dimensional reduction by means of Variational Multiscale Method

(VMS) and apply Variational Consistent Dimensional Reduction to characterize effective material parameters, comparing the fluid permeability (from solving Stokes flow on the resolved sub-scale) and Chloride diffusion properties (from solving Fickian diffusion) of the cracked material at different stages of healing.

References:

[1] Reinhardt, H.W. et al. Recovery against Environmental Action. In: de Rooij, M. et al. Self-Healing Phenomena in Cement-Based Materials. Vol. 11, pp. 65-117, Springer, Dordrecht (2013).

[2] Ma, H., Yi, C., Wu, C. Review and outlook on durability of engineered cementitious composite (ECC). In: Construction and Building Materials. Vol. 287, pp. 122719 (2021).

[3] Buegger, U., Tofeti-Lima, T., and Jänicke, R. Analysis of the self-healing capacity of ECCs with high levels of cement replacement by limestone calcined clay cements (LC3), based on micro X-ray computed tomography (µXRCT). In: MATEC Web of Conferences. Vol. 409. EDP Sciences (2025).

**Thin-walled beams from Naghdi models**

Ljulj, Matko; Tambača, Josip
*Faculty of Science, University of Zagreb, Croatia*

15:40

In this talk, a derivation of elastic thin-walled beams in the context of linear elasticity will be presented. We observe a family of bodies of the form [0,L] x $\varepsilon S^{\varepsilon}$, where L is the beam length and $S^{\varepsilon}$ is an $\varepsilon$-thick strip around a curve M : [0,l] -> R. We seek the limit as $\varepsilon \to 0$. We approach the problem in two ways: firstly, bodies are modeled as thin elastic shells of the Naghdi type with thickness $\varepsilon^2$, and secondly, bodies are modeled as thin elastic rods of the Naghdi type with a cross-section dependent on $\varepsilon$. The Naghdi-type models used in the analysis are those for shells and rods with lower regularity, analyzed by the same authors in their previous works. In both approaches, we let $\varepsilon \to 0$, determine the limit, and compare it with results obtained in the literature.

## S08.08: Homogenization

Date: March 19, 2026 17:30–18:30
Room: KI, M11.42
Chair(s): Eidel, Bernhard
Eisenträger, Johanna

**Energetically Consistent Nano-Micro Scale Transition by Computational Homogenization Using Molecular Statics RVEs in a micro-FEM**

Neelakandan, Aagashram (1); Albe, Karsten (2); Eidel, Bernhard (1)
*1: Technische Universitat Bergakademie Freiberg, Germany*
*2: Technische Universitat Darmstadt, Germany*

17:30

We present a two scale computational homogenization framework that carries atomistic accuracy to micrometer scale structures. The upper scale is a microscale finite element model, while the lower scale is a nanoscale representative volume element solved with molecular statics. The scale transition follows Hill macrohomogeneity and is expressed using power conjugate stress and strain measures. For finite deformations, the microscale boundary value problem is formulated in a total Lagrangian setting using the second Piola Kirchhoff stress and the Green Lagrange strain. At the nanoscale, volume averaged Cauchy stresses are obtained from LAMMPS and then mapped consistently to the second Piola Kirchhoff stress through rotation and pull back operations. The required microscale consistent tangent is computed with forward differences based on symmetric perturbations of the right stretch tensor from polar decomposition. This total Lagrangian formulation naturally separates the tangent into material and geometric contributions. The approach is nanoscale material agnostic, and we illustrate its use with face centered cubic metals modeled using embedded atom method potentials.

**X-FFT: Computational homogenization of 3D elasticity with the accuracy of interface-conforming FEM and the speed of FFT methods**

Gehrig, Flavia (1); Schneider, Matti (1,2,3)
*1: University of Duisburg-Essen, Institute of Engineering Mathematics*
*2: Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern*
*3: Center for Nanointegration Duisburg-Essen (CENIDE)*

17:50

Computational homogenization methods based on the fast Fourier transform (FFT) are renowned for their numerical efficiency and stability. However, traditional discretizations come with compromised accuracy - due to the regular grid, material interfaces cannot be resolved accurately, in general.
To address this limitation, we developed a novel FFT-based solver for three-dimensional linear elastic unit-cell problems, leveraging the extended finite element (X-FEM) discretization with modified absolute enrichment. X-FEM effectively resolves weak discontinuities at material interfaces through additional shape functions, thereby providing local strain and stress fields which are accurate up to the interface. To mitigate the conditioning issues characteristic for traditional X-FEM implementations, we propose a preconditioner based on strongly stable GFEM. Computational studies demonstrate that our X-FFT solver achieves superior accuracy, numerical efficiency, and stability when solving three-dimensional linear elastic homogenization problems with smooth interfaces.

**Neural Network Compression for Computational Polyconvexification of Isotropic Functions**

Balazi, Loïc; Neumeier, Timo; Peter, Malte A.; Peterseim, Daniel; Salmon, Julian
*University of Augsburg, Germany*

18:10

When simulating non-convex variational problems in finite-strain damage and phase transition models, one encounters significant challenges arising from the lack of convexity, including non-existence of minimisers, mesh sensitivity, and numerical instabilities. Relaxation via semi-convexification provides a consistent variational framework that guarantees the existence of minimisers and mesh-independent approximations, while simultaneously revealing microstructural information in a multiscale sense. However, the concurrent computation of semi-convex envelopes within finite element simulations is computationally expensive, motivating the development of efficient offline–online compression strategies.
In this talk, we present a structure-preserving neural network compression approach for computationally determined polyconvex envelopes of isotropic functions. The approach builds on the dimension-reduced characterisation of polyconvexity using signed singular values and exploits symmetry and monotonicity properties rooted in Ball's polyconvexity criterion. Feasibility, accuracy, and performance are demonstrated through numerical experiments, showing substantial compression and computational speed-up while preserving the underlying theoretical structure.

## S09: Laminar flows and transition

Organizer(s): Schlatter, Phillip *(nan)*
Örlü, Ramis *(OsloMet - Oslo Metropolitan University)*

## S09.01: aminar flows and transition

Date: March 19, 2026 14:00–16:00
Room: KII, M17.72

### Aspects of the laminar and transitional flow in curved and helical pipes

Schlatter, Phillip 14:00
*FAU Erlangen-Nürnberg, Germany*

Curved pipes are probably more the rule than the exception, be it helical or toroidal, or simply spatial bends. Many studies have focused on the properties of straight pipes, e.g. related to stability, transition and turbulence. However, even small amounts of curvature affect the laminar state and the turbulent mean flow alike. The most visible flow structures are the so-called Dean vortices due to the imbalance of the pressure forces. This new base flow will change e.g. the stability properties (a flow in a bent pipe is always modally unstable as we will show), transition is affected (there is an interesting interaction between modal and non-modal instability), and finally even turbulence properties change (one can even find a region of sublaminar drag). Helically bent pipes will even break the symmetry of the Dean vortices, making the flow more complex and less studied. In this talk, we will try to summarise some of the recent findings in our studies of bent pipes, hopefully appealing to both engineering and fundamental audiences.

### Convection in an internally heated dielectric fluid layer

Nagaraj, Kushal; Szabo, Peter; Egbers, Christoph 14:40
*Brandenburg University of Technology, Germany*

Convection in polar dielectric fluids can be caused by dielectric losses if the fluid is exposed to an alternating electric field causing internal heating. In contrast to a microgravity environment where only the dielectrophoretic (DEP) force drives TEHD convection, laboratory conditions introduce a competing interaction between electric forcing and Archimedean buoyancy causing natural convection. To investigate this particular interaction, three-dimensional (3D) direct numerical simulations (DNS) are performed for the polar dielectric fluid 1-Nonanol at 50 Hz, characterised by a large Prandtl number, Pr, and a large dielectric loss factor. The working fluid is confined between two horizontal boundaries that are maintained at the same constant temperature, while internal heating arises from dielectric losses caused by an alternating electric field from within.
The DNS simulations reveal a sequence of convective regimes when the applied electric potential is increased. At small electric forcing, Archimedean buoyancy dominates and the flow resembles classical Rayleigh-Benard convection, with large-scale roll structures spanning the layer. With increasing electric potential, regimes emerge in which the DEP force and Archimedean buoyancy compete. This alternates the convective structure from Benard cells giving rise to localised TEHD convection from hexagonal to rectangular patterns. At stronger electric forcing, irregular time-dependent convection develops indicated by plume detachment and deep convection.
Analysis of the thermal and kinematic boundary layers shows that the thermal boundary layer thickness maintains scaling properties consistent with buoyancy-driven convection. In contrast, the velocity field is strongly affected by electric forcing, with clear differences observed between flows dominated by Archimedean buoyancy and those dominated by the dielectrophoretic (DEP) forces. This behaviour can be explained by the different ways buoyancy and electric forces drive the flow. Scaling relations for the Nusselt number, internal and kinetic energy densities are consistent with boundary-driven flows. Comparisons with internally heated convection show similar transport behaviour but also highlights the unique role of the inter-

nal dielectric heating source.
These results offer new insights into dielectric heated internal convection their driving mechanism and clear differences to Archimedean buoyancy dominated flows. The underlying convective dynamics show how the two competing forces, buoyancy and DEP force, can change the overall fluid flow behaviour. The results also support recent experimental studies by Strangfeld et al., highlighting the importance of combining simulations with laboratory experiments to better understand convection driven by both the DEP force and Archimedean buoyancy.

**Hydrodynamic stability of MHD fluid through rotating rectangular porous channel**

Kumar yadav, Satyendra 15:00
*Motilal Nehru National institute of technology allahabad, prayagraj, India*

This work explores the influence of a transverse magnetic field on the Poiseuille flow of an electrically conducting fluid through a porous medium confined between two rotating infinite parallel plates. Using the Chebyshev collocation technique, the generalized Orr-Sommerfeld equations are solved to determine the wave number and perturbation growth rate. The analysis shows that flow instability is significantly governed by the interplay between magnetic effects and porous resistance. An increase in Reynolds number enhances instability by amplifying perturbation growth, while the transverse magnetic field exhibits a stabilizing effect for specific porous configurations. These findings emphasize the stabilizing role of magnetism in electrically conducting fluid flows through porous media.

**Investigation of the flow topology in the mouth of a filter feeding-fish – a CFD study towards a non-clogging technical filtration device**

Hormozi, Hiva; Baars, Albert 15:20
*Hochschule Bremen, City university of applied sciences, Germany*

Filter-feeding fishes such as mackerel or paddlefish obtain food particles through passive water filtration while maintaining a non-clogging filter system. As part of the EU project Nature4Nature we aim to investigate the flow topology inside the fish mouth to understand the physical principles underlying this filtration mechanism and to use this knowledge to design a potential non-clogging filter model for technical applications using computational fluid dynamics (CFD). However, the relatively complex geometry of biological species, together with the presence of structures spanning multiple length scales, makes flow simulations computationally demanding. As a result, the present study has been divided into two parts.

In the first part, the inner and outer geometry of the mouth is described using mathematical functions, enabling reproducible and systematic parameter variations. In a parallel study, the pressure drop induced by the presence of gill rakers - which act as a sieve within the mouth cavity - is investigated as a function of Reynolds number and geometrical parameters and described using the Darcy–Forchheimer relation. This relation is then implemented in the first part of the simulation to account for the pressure drop caused by the gill rakers in the form of a porous-medium model. The numerical simulations are carried out using structured grids and OpenFOAM solver.

In this work, an abstracted two-dimensional mouth geometry of a mackerel is investigated at a Reynolds number of 15,000, which results in steady laminar flow with negligible flow separation and a mean inlet velocity consistent with values reported in the literature. The volume flow rates between the gill arches are analyzed and are found to depend strongly on the curvature of the mouth walls, while boundary-layer effects influence the distribution of volume flow through the gill slits. No cross-flow filtration is observed, contrary to what has been hypothesized in the literature.

## S10: Turbulence and reactive flows

Organizer(s): Beck, Andrea *(Universität Stuttgart)*

## S10.01: Turbulence and reactive flows

Date: March 18, 2026 14:00–16:00
Room: KII, M17.72
Chair(s): Schumacher, Jörg

### Passive Scalar Intermittency at High-Reynolds Numbers : A first Perspective from ODT

Joshi, Abhishek (1,2); Klein, Marten (1,2); Schmidt, Heiko (1,2) 14:00
*1: Brandenburg Technological University Cottbus - Seftenberg, Germany*
*2: Scientific Computing Lab, Energie-Innovationszentrum Cottbus*

Passive scalar turbulence exhibits strong anomalous scaling, with structure function exponents $\zeta_n$ deviating significantly from the K41 dimensional predictions due to intermittency. DNS has successfully quantified these deviations across a range of Reynolds numbers, but its computational cost limits extensive parameter studies such as Schmidt number (Sc) scaling. One-Dimensional Turbulence (ODT) offers a computationally efficient alternative through full-scale resolution of turbulent mixing along a one-dimensional domain. Turbulent advection is modeled by stochastically sampled mapping events that punctuate deterministic flow evolution, formulated on conservation principles and turbulence phenomenology. An energy-based rejection method samples events from an evolving distribution function. However, ODT's ability to capture scalar intermittency statistics at high Reynolds numbers requires systematic validation. To maintain flow isotropy while driving sustained turbulence, we implement a stochastic forcing scheme for ODT. Passive scalar fluctuations are evolved under a uniform mean gradient for $Sc = 1$. ODT simulations are performed up to $Re_\lambda \approx 280$ using ensemble realizations to achieve statistical convergence of high order moments. Scalar structure functions $T_n(r) = \langle|\theta(x+r) - \theta(x)|^n\rangle$ are computed for orders $n = 2$ to $10$. Scaling exponents $\zeta_n$ extracted from inertial range scaling are compared with DNS benchmarks, demonstrating the expected anomalous behavior with increasing deviation from Kolmogorov-Obukhov predictions ($\zeta_n = n/3$) at higher orders. Compensated structure function plots confirm extended scaling ranges. Additionally, probability density functions (PDFs) of scalar dissipation rate $\chi$ exhibit the characteristic stretched exponential tails indicative of strong intermittency, with tail statistics compared with DNS observations. The convergence of both structure function moments and dissipation PDFs across ensemble realizations confirms adequate statistical sampling of rare, intense fluctuation events. These preliminary results validate ODT for passive scalar intermittency. These results demonstrate ODT's capability to reproduce intermittency statistics at reduced computational cost, making it a promising approach for extended parametric studies of passive scalar turbulence.

### Influence of Spanwise Curvature and Thermal Boundary Conditions on Heat Transfer in Turbulent Annular Pipes

Tsai, Pei-Yun; Klein, Marten; Schmidt, Heiko 14:20
*BTU Cottbus-Senftenberg, Germany*

Turbulent flow and heat transfer in concentric coaxial (annular) pipe configurations have been studied for decades using numerical and experimental approaches. However, accurately resolving high Reynolds number turbulent flow and heat transfer across a range of Prandtl numbers, particularly in the presence of wall curvature, remains challenging. In this work, heat transfer, treated as a passive scalar in pressure-driven annular pipe flow, is investigated using the stochastic one-dimensional turbulence (ODT) model [1].

ODT is a dimensionally reduced model that makes it feasible to resolve all relevant turbulent scales of the flow along a single radial coordinate. Turbulent advection is modeled by a stochastically sampled sequence of spatial mapping events. The applicability of ODT to heated channel has been established

in prior studies [2,3,4], and is here extended to concentric annular coaxial pipe flows with different boundary conditions.

In this study, we specifically examine the effects of different thermal boundary conditions and Prandtl numbers on annular pipe flow, with a particular focus on how spanwise curvature influences the thermal boundary layer and overall thermal behavior. Two heating conditions are considered: uniform heat flux and constant temperature difference between the inner and outer cylinder walls, respectively. We show that stochastic modeling aligns well with classical mixing-length theory. By extending conventional boundary layer theory to account for spanwise curvature, we analyze how wall-curvature-induced asymmetry develops between the inner and outer thermal boundary layers, resulting in characteristic dependencies on both Reynolds and Prandtl numbers.

**References**

[1] A. R. Kerstein, Journal of Fluid Mechanics **392**, 277 (1999).

[2] M. Klein, H. Schmidt, and D. O. Lignell, International Journal of Heat and Fluid Flow **93**, 108889 (2022).

[3] P.-Y. Tsai, H. Schmidt, and M. Klein, PAMM **23**, e202300167 (2023).

[4] P.-Y. Tsai, H. Schmidt, and M. Klein, PAMM **25**, e70006 (2025).

**Heat transfer enhancement by surface roughness in impinging jets**

Elsner, Ferdinand (1); Häber, Thomas (2); Moosmayer, Sebastian (4); Secchi, Francesco (6); Suntz, Rainer (5); Raiola, Marco (3,1); Trimis, Dimosthenis (4); Gatti, Davide (1); Frohnapfel, Bettina (1)

*1: Institute of Fluid Mechanics, Karlsruhe Institute of Technology, Germany*
*2: Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology, Germany*
*3: Department of Aerospace Engineering, Universidad Carlos III de Madrid (UC3M), Spain*
*4: Engler-Bunte-Institut Combustion Technology (EBI-CT), Karlsruhe Institute of Technology, Germany*
*5: Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology, Germany*
*6: Institute for Water and Environment (IWU), Karlsruhe Institute of Technology, Germany*

14:40

Impinging jets are widely employed in technical applications for cooling purposes. However, the role of surface roughness in enhancing heat transfer is not yet fully understood. A key reason is the scarcity of systematic experimental studies investigating the influence of wall roughness on convective heat transfer. Therefore, this study aims to investigate the heat transfer characteristics of an impinging jet emerging from a circular nozzle as a fully developed turbulent flow. Measurements are carried out through a "gradient sensor", allowing to solve for the convective heat transfer from the impingment surface temperature measured by infrared thermography. Heat transfer is investigated using both smooth and rough impingement plates. Two different rough surfaces with identical roughness characteristics but varying mean roughness heights are being measured. Heat transfer measurements are carried out for various jet flow velocities to obtain the local Nusselt number (Nu) distribution as a function of the radial distance from the impingement center. This is performed for varying Reynolds numbers (Re) and nozzle-to-plate distances. The impingement plate is heated by pumping thermal oil at constant temperature through a heating coil underneath the plate. An infrared camera measures the surface temperatures of the impingement plate. From the difference of the surface temperature and the oil temperature, the local wall heat flux can be derived. To get meaningful heat flux data from the plate into the flow, it is found that the impact of radial conduction within the impingement plate must be accounted for in this evaluation. Radial distributions of Nu are obtained by averaging the heat flux along the circumferential coordinate and converted into Nu. The measured Nu for the smooth plate is found to agree well with results from Direct Numerical Simulation (DNS) studies, which are limited to the low Re range. Interestingly, roughness does not influence the Nu-distribution in the Re-range that is accessible by DNS. However, the experimental results demonstrate a significant increase in Nu due to surface roughness at higher Re. Furthermore, the radial distribution of Nu over a rough surface compared to a smooth one is found to change in a way that indicates a reduced sensitivity of the local heat transfer to large-scale flow motions further away from the impingement plate for the rough impingement plate.

**Small-scale statistics and structures in compressible homogeneous isotropic turbulence**
Alam, Shadab (1); Zinchenko, Georgy (1); Federrath, Christoph (2); Schumacher, Jörg (1) 15:00
*1: TU Ilmenau, Germany*
*2: ANU Canberra, Australia*

Compressible turbulence introduces additional layers of complexity through new mechanisms, which are absent in its incompressible counterpart. This includes shocklets and shocks, dilatational strain and thermodynamic interactions. These structures and processes shape the dynamics of systems ranging from the interstellar medium to engineering applications, such as gas turbines and supersonic propulsion. We are interested in the small-scale statistics in compressible turbulence for both, the subsonic and supersonic regimes. Our investigations are based on direct numerical simulations of compressible homogeneous isotropic turbulence for turbulent Mach numbers between 0.1 and 10 and moderate Reynolds numbers. The flow is in a statistically steady regime, which is sustained by a solenoidal volume forcing. We report scaling laws of moments of the kinetic energy dissipation rate and its components with respect to the Reynolds number, investigate deviations in the scaling from the incompressible case, and identify the vortex- and shear layer-structures which are responsible for the statistics.

**On random field modeling of anisotropic synthetic turbulence**
Antoni, Markus; Lindner, Felix 15:40
*Universität Kassel, Germany*

Stochastic methods for the generation of synthetic turbulent velocity fields are widely used in the context of RANS and LES simulations. Examples include the superposition of stationary RANS calculations by artificial spatio-temporal fluctuations or the generation of interface data and boundary conditions for hybrid methods. The employed stochastic models are often based on stochastic spectral representations and are usually designed to be compatible with prescribed statistical flow properties such as Reynolds stress anisotropy. However, available anisotropic models typically have shortcomings such as incompatibility with Kolmogorov's hypothesis of local isotropy or a lack of invariance with respect to the choice of the underlying coordinate frame. In this talk we present a refined random field model that overcomes these difficulties and can be simulated efficiently.

## S10.02: Turbulence and reactive flows
Date: March 18, 2026 16:30–18:30
Room: KII, M17.72
Chair(s): Beck, Andrea

**Aspects of a highly reduced order model for turbulent mixing based on hierarchical swapping of fluid parcels**
Starick, Tommy (1); Schmidt, Heiko (1,2) 16:30
*1: BTU Cottbus-Senftenberg, Germany*
*2: Scientific Computing Lab (SCL), Energy Innovation Center (EIZ), BTU Cottbus-Senftenberg, Germany*

Turbulent mixing is a ubiquitous phenomenon that plays a crucial role in a wide range of industrial applications involving turbulent liquid or gaseous flows. The Hierarchical Parcel-Swapping (HiPS) model developed by A.R. Kerstein [J. Stat. Phys. 153, 142-161 (2013)] represents a computationally efficient and scale-resolving turbulent mixing model, which reproduces the effects of turbulence on time-evolving, diffusive scalar fields. In HiPS, the diffusive scalar fields or a state space is interpreted as a binary tree structure, which is an alternative approach compared to the most common mixing models. The binary tree, consisting of nodes, extends from the integral length scale at the top level down to the smallest represented scales at the bottom level, where the nodes are interpreted as individual fluid parcels. Each intermediate level is also associated with a characteristic length scale and time scale. Length scales decrease geometrically from level to level, and the corresponding time scales are determined according to turbulence inertial-range scaling. The state variables are solely located at the bottom level of the tree. To represent the effects of turbulent advection, HiPS employs

stochastic swaps of sub-trees at rates determined by the turbulent time scales associated with each sub-tree. Mixing occurs only when swaps are performed on individual parcels, since this alters their relative proximity. Recently, the HiPS formulation was generalized to handle variable Schmidt numbers, enabling the study of scalar power spectrum scalings and scalar dissipation statistics [J. Fluid Mech. 1020, A13 (2025)]. Direct tracking of fluid parcels further allows HiPS to compute Richardson pair dispersion and scalar structure functions, addressing anomalous scaling attributed to intermittency. Furthermore, HiPS is employed as a mixing model in transported Probability Density Function (PDF) methods to mitigate the main shortcomings of the most commonly used mixing models. In the talk, we will summarize the state of the art and highlight current research activities.

**Buoyancy-shear coupling in One-Dimensional Turbulence: from Rayleigh–Bénard to mixed convection**

Li, Hanchen (1,2); Klein, Marten (1,2); Schmidt, Heiko (1,2); Hoffmann, Fabian (3) 16:50

*1: Chair of Numerical Fluid and Gas Dynamics, Brandenburg University of Technology Cottbus-Senftenberg, Cottbus, Germany*
*2: Scientific Computing Lab (SCL), Energy Innovation Center (EIZ), Brandenburg University of Technology Cottbus-Senftenberg, Cottbus, Germany*
*3: Institut für Meteorologie, Freie Universität Berlin, Berlin, Germany*

One-dimensional turbulence (ODT) is a single-column model that explicitly resolves molecular transport along a 1D vertical domain, while modelling turbulent advection via stochastically sampled spatial mappings ("eddy events"). Previous studies have shown ODT's capability to represent turbulent shear convection and Rayleigh-Bénard convection, but buoyancy-coupled shear flows remain less explored.
Here, we present an ODT formulation for turbulent buoyant flows and assess it on two canonical cases. First, we formulate Rayleigh-Bénard convection under the simple Boussinesq approximation and compare results with previous studies. Then, we extend the problem to Poiseuille-Rayleigh-Bénard convection (mixed convection), identify the key weaknesses in ODT's turbulence closure for buoyant flows, and propose an empirically motivated modification of the eddy events.
This study provides building blocks for ongoing extensions of ODT towards atmospheric boundary-layer applications, especially boundary layers topped by stratocumulus clouds, which are a crucial element of the climate system by exerting a substantial negative (i.e., cooling) forcing on Earth's radiation budget. Since these boundary layers are difficult to model at the resolutions used in weather and climate prediction models, in part due to sharp capping inversions and cloud-top entrainment, ODT may offer a computationally efficient framework to understand the coupled buoyancy-shear-entrainment processes.

**Algorithmic construction of reduced-order reactor network models based on CFD data**

Gossel, Lisanne (1,2); Berkel, Leon Loni (3); Gauges, Maira (3); Brand, Paul (1); Fricke, Mathis (1); Hasse, Christian (3); Stagni, Alessandro (4); Nicolai, Hendrik (3); Bothe, Dieter (1); Faravelli, Tiziano (4) 17:10

*1: Institute for Mathematical Modeling and Analysis, TU Darmstadt, Darmstadt, Germany*
*2: Institute for Numerical Methods in Fluid Mechanics, TU Darmstadt, Darmstadt, Germany*
*3: Institute for Simulation of Reactive Thermo-Fluid Systems, TU Darmstadt, Darmstadt, Germany*
*4: CRECK Modeling Group, Politecnico di Milano, Milan, Italy*

In search for an energy storage material, which enables future renewable energy supply on a global scale, metal powders recently gain growing interest in energy science and engineering as a recyclable chemical energy carrier [1]. Metal dust combustion in chemical reactors is one of the core processes to this new technology. Experimental studies and CFD (e.g., [2]) support the understanding of the fundamental fluid physics within the reactor, however, coupling these models to detailed chemistry including thousands of reactions is usually computationally prohibitive. One way to overcome this are Chemical Reactor Network (CRN) models [3], a physics-based reduced-order method to describe chemical reactors. CRNs are graph-like representations of the full reactor, where idealized modeling reactors representing a certain region and physico-chemical state of the reactor sit at the nodes, while the edges of the network hold information on the mass fluxes between

the different compartments. Compared to CFD simulations, CRNs are highly efficient, and thus enable detailed chemistry computations, for example to investigate the formation of pollutant species like NOx. Moreover, their high efficiency allows integrating CRNs into multi-query tasks like process optimization.
CRNs can be understood as a post-processing method for CFD (RANS or LES). The present contribution focuses on recent achievements in developing algorithms for automatically creating CRN models based on primary CFD data. Algorithmic CRN construction supports robust and reproducible CRN models and helps tapping the potential in time efficiency of the method. Moreover, the embedding of the modeling process into the algorithms advances the CRN methodology itself since bottlenecks for the modeling are easier revealed. One key aspects of any such algorithms is the division of the reactor domain into functional compartments. In this regard, a new algorithm that puts a large emphasis on model consistency is introduced. The newly developed algorithm shows good performance and robustness independently of particular features of a certain testcase. A tractable model complexity is achieved while maintaining a physically consistent model of the reactor. The key modeling aspects of the introduced algorithms for CRN construction will be discussed, emphasizing the importance of properly capturing both, mean characteristics of the flow as well as turbulence and mixing. The usage of CRNs in complement to CFD will be exemplified.

[1] Bergthorson, J. et al. (2015). Applied Energy, 160, 368-382.
[2] Steffens, P. et al. (2025). Fuel, 392, 135205.
[3] Trespi, S. et al. (2020). Energy & Fuels, 35(9), 7121-7132.

**Synthesizing atmospheric boundary-layer turbulence by stochastic modeling and multi-scale filtering**

Klein, Marten (1,2); Zenker, Christian (3); Oevermann, Michael (3); Schmidt, Heiko (1,2)
*1: Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus-Senftenberg, Germany*
*2: Scientific Computing Lab, Energie-Innovationszentrum Cottbus, Germany*
*3: Fachgebiet Numerische Mathematik und Wissenschaftliches Rechnen, BTU Cottbus-Senftenberg, Germany*

17:30

Aeroelastic simulation tools offer a dynamical, reduced-order modeling framework for the simulation of full-scale wind turbines. These tools yield power output, rotor torque, structural stresses and deformations in response to a prescribed wind field based on physical assumptions. In-plane and out-of-plane load moments are computed for the wind turbine rotor by combining blade-level boundary-element-based modeling, originally developed for propellers, with a wake model to represent the momentum extraction. The modeling framework has the capability to capture unsteady wind stress distributions across the rotor blades that arise from wind velocity fluctuations in turbulent wind fields. Putting simplifying aerodynamic assumptions aside, a key limitation of the modeling framework remains in the representation of the turbulent inflow in terms of the atmospheric boundary layer (ABL). The ABL is characterized by intricate spatio-temporal correlations and exhibits intermittent dynamics that depend on the flow regime and manifest themselves by sudden extreme events, like wind gusts. State-of-the-art modeling of ABL turbulence utilizes random sampling from observed wind speed distributions, heuristically extended and spectrally enriched by selected statistical features. It is unclear at present to which extent short-term load fluctuations can be captured by the heuristic approaches that lack causality and physical processes.

This work addresses some open issues related to capturing emerging intermittency features in turbulent ABLs with the objective to potentially enhance the modeling capabilities of aeroelastic simulation tools. The problem boils down to synthesizing a three-dimensional 'frozen-in' turbulence box. For this purpose it is proposed to utilize a map-based stochastic, so-called one-dimensional turbulence (ODT) model to generate vertical-temporal correlations by evolving an ensemble of instantaneous flow profiles, replacing some heuristic assumptions. A time-to-space transformation is applied to each ensemble member to obtain streamwise-vertical sections of the turbulent box. These sections are finally correlated in lateral (spanwise) direction by application of a multi-scale filter, making use of low-order statistics obtained from reference data. In the contribution, the modeling approach will

be discussed in more detail with comparison to reference data in order to highlight benefits and remaining limitations.

## S10.03: Turbulence and reactive flows

Date: March 19, 2026 08:30–10:30
Room: KII, M17.72
Chair(s): Beck, Andrea

### Toward a unified data-driven turbulence model through multi-objective learning

Liu, Zhuoran; Wang, Haochen; Zhao, Zhuolin; Xiao, Heng 08:30
*University of Stuttgart, Germany*

Turbulence is among the last unresolved problems of classical physics and remains a major bottleneck to accurate flow prediction in climate, aerospace, and energy systems. Industrial simulations rely on averaged representations of turbulence, which often struggle to predict flows governed by multiple interacting mechanisms. We present a unified, data-driven turbulence modeling framework based on multi-objective learning to achieve enhanced performance across diverse flow regimes. The resulting *unified foundation model*, trained on five representative flows, adapts seamlessly across regimes without manual intervention. It surpasses existing turbulence models across a broad spectrum of canonical flows and maintains improved performance in realistic three-dimensional configurations of industrial relevance, including generic car and gas turbine diffuser. For targeted applications, *specialist models* trained on tailored datasets further enhance accuracy. These results demonstrate the feasibility of a deployable, generalized turbulence model that unifies multiple flow mechanisms within a single architecture for broad scientific and industrial applications.

### CFD modeling of aerosol removal in pool scrubbing using an Euler–Euler approach

Li, Shiwang; Liao, Yixiang 08:50
*Helmholtz-Zentrum Dresden-Rossendorf, Germany*

Pool scrubbing is an important mitigation measure for reducing radioactive aerosol release during nuclear reactor accident conditions. Its removal efficiency is governed by the coupled effects of bubble dynamics and aerosol transport within rising bubbles. Among the mechanisms contributing to aerosol removal, centrifugal impaction, gravitational sedimentation, and Brownian diffusion are dominant. Computational fluid dynamics (CFD) provides a promising tool for investigating these complex, interacting processes; however, detailed CFD studies addressing aerosol removal in pool scrubbing remain scarce.

In this work, a numerical investigation of aerosol removal in pool scrubbing is conducted using an Euler–Euler multi-fluid framework, with particular emphasis on the modeling of interphase momentum transfer and particle removal mechanisms. Drag is the dominant contribution to momentum exchange between the gas and liquid phases and strongly influences bubble rise velocity, residence time, and, consequently, aerosol removal efficiency. The results show that the effective drag coefficient is significantly reduced under pool scrubbing conditions. Classical drag models, such as the Ishii–Zuber and Tomiyama models, which perform well in pipe flows and bubble columns, tend to underpredict bubble rise velocities in pool scrubbing columns. This deficiency is attributed to their inability to account for strong turbulence induced by high gas injection velocities and large bubble sizes. Motivated by recent findings of Salibindla et al. (J. Fluid Mech., 2020), a modified drag model is proposed, resulting in improved predictions of bubble rise velocity and void fraction distributions.

Aerosol particles in the gas and liquid phases are treated as separate species, and particle removal is modeled as a mass transfer process from gas to liquid. Based on the improved hydrodynamic description, four aerosol removal models from the literature (Fuchs, Kunsek, Powers, and Fujiwara) are evaluated over a range of particle sizes. The results demonstrate a strong particle-size dependence of model performance. Models accounting for bubble deformation provide reasonable agreement for small particles but overpredict removal for larger particles, while spherical-bubble-based models generally underpredict removal. To address this limitation, a particle-size-dependent correction

factor is introduced into the centrifugal impaction term of the Powers model, leading to significantly improved predictions across all test cases.

**Dependency of the transitionally rough regime on planform and frontal solidity**

Busse, Angela; Zhdanov, Oleksandr 09:10
*Technische Universität Berlin, Germany*

The effects of rough walls on wall-bounded turbulent flows are known to be strongly dependent on the height of the roughness but is also significantly affected by the roughness topography, i.e., the shape and distribution of the features of the rough surface. The topography-dependence of the fluid dynamic roughness effect of a surface encompasses two key points: Firstly, the equivalent sand-grain roughness of a surface, which is measured in the fully rough regime in reference to Nikuradse's sand-grain roughness, depends not only on the physical roughness height, but also on topographical parameters such as the planform and frontal solidity. Secondly, in the transitionally rough regime, non-universal behaviour is observed even after suitable scaling with the equivalent sand grain roughness of the surface. It is yet to be fully understood how the non-universal behaviour in the transitionally rough regime depends on the surface topography.

In the present study, the focus is placed on the second point, and the aim is to investigate the dependency of the transitionally rough behaviour of regular rough surfaces on two topographical parameters, namely planform and frontal solidity, which are widely used to characterise the topography of regular roughness. To this end, direct numerical simulations of turbulent channel flow have been conducted for a series of rough surfaces constructed from pyramid-shaped roughness elements that allow the independent variation of the investigated topographical parameters. Simulations have been conducted for a range of Reynolds numbers for each case to establish the transitionally rough behaviour of each surface. In this contribution, the dependency of the transitionally rough behaviour on the planform and frontal solidity will be discussed using both mean flow and turbulence statistics and compared with the transitionally rough behaviour of other surface types, such as multi-scale irregular roughness and clustered roughness.

**Exploring the Impact of Methanol-Assisted Reactivity Stratification on Ammonia combustion**

Hemaizia, Abdelkader (1); Abdelsamie, Abouelmagd (1); Verma, Rakhi (2); Mauss, Fabian (2); Thévenin, Dominique (1) 09:30
*1: 1Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke", Universitätsplatz 2, Magdeburg, 39106, Germany.*
*2: 2Department of Thermodynamic/Thermal Process Engineering, BTU Cottbus-Senftenberg, Cottbus, 03046, Germany.*

The need to decarbonize large-scale combustion systems has positioned ammonia as a promising zero-carbon fuel. However, its poor combustion reactivity characterized by slow flame speed, high ignition energy, and limited radical production limit its practical use in engines. Blending NH3 with hydrocarbons and/or reactive oxygenated fuels such as alcohols introduces additional radicals (like H and OH), enhances flame propagation, and reduces ignition delay, providing a feasible pathway toward stable and low-carbon combustion. Despite the growing interest in NH3-based fuels, studies on NH3 blended with lower alcohols such as methanol (CH3OH) remain scarce. This work investigates the flame characteristics of NH3/CH3OH blended fuels, with a focus on how local mixture stratification influences flame stabilization and NOx formation pathways under different operating conditions. Using detailed chemical kinetics and one-dimensional flame configurations, we quantify the impact of stratification intensity, equivalence ratio, and blend ratio on heat release, radical distribution, flame speed, and the relative contribution of the thermal, NNH, and HNO pathways to global NO formation. The results are expected to demonstrate that introducing reactive stratification can enhance flame propagation and stabilization while reducing NO formation rates commonly associated with CH3OH addition. Overall, this study will provide critical insights into a novel strategy for overcoming ammonia's combustion challenges and offers a pathway toward more practical, efficient, and cleaner decarbonized combustion system.

**Kinetic Modeling and Simulation-Based Optimization of $CO_2$ Hydrogenation reactions to produce Methanol**

Sindhav, Vishal Govindbhai (1); Verma, Rakhi (1); Günther, Vivien (2); Hemaizia, Abdelkader (3); Thévenin, Dominique (3); Mauss, Fabian (1)

*1: Chair of Thermodynamic/Thermal Process Engineering, Brandenburg University of Technology Cottbus-Senftenberg, 03046 Cottbus, Germany*
*2: LOGE AB, Cottbus, 03044, Germany*
*3: Laboratory of Fluid Dynamics and Technical Flows, University of Magdeburg "Otto von Guericke", Universitätsplatz 2, Magdeburg, 39106, Germany*

09:50

Researchers worldwide are making significant efforts to reduce $CO_2$ concentrations, as greenhouse gases, particularly carbon dioxide ($CO_2$) pose a major global challenge. One effective way to do this is by converting $CO_2$ into methanol through a hydrogenation reaction. Methanol is widely used in many industries and also has potential as a fuel additive and energy source. Therefore, converting $CO_2$ into methanol provides a dual benefit by reducing carbon emissions while producing a value-added chemical. This study investigates the kinetics of $CO_2$-to-methanol synthesis and aims to optimize it using a model-based simulation approach to achieve maximum $CO_2$ conversion at lower operating temperatures. The main emphasis of this work is the development and application of a kinetic model to describe $CO_2$ hydrogenation over copper-based catalysts under controlled operating conditions. The effect of temperature on reaction kinetics and methanol formation will be examined by simulating the process at five temperatures: 503 K, 523 K, 543 K, 563 K, and 583 K. These temperatures are selected based on performance trends reported in the literature. Kinetic expressions derived from the Arrhenius equation will be used to evaluate the influence of activation energy (E) and pre-exponential factors (A) on reaction rates. Literature reported kinetic parameters and experimental reference data will be employed to validate the kinetic model and ensure realistic prediction of reaction behaviour. Particular attention will be given to studies reporting a maximum $CO_2$ conversion of 12.1% at 523 K and 28 atm using a $Cu/ZnO/ZrO_2/MgO/\gamma\text{-}Al_2O_3$ catalyst. Based on this literature case, the simulations will assess whether similar or improved $CO_2$ conversions can be achieved at lower temperatures through kinetic optimization. Sensitivity analyses will be carried out by changing values of activation energies and rate constants within physically meaningful ranges to identify the most influential kinetic parameters governing $CO_2$ conversion and methanol yield. This approach will help determine dominant reaction pathways and temperature regions that favour methanol synthesis, as well as conditions that limit overall conversion. The expected outcome of this study is the identification of optimal temperature ranges and kinetic parameter combinations that maximise $CO_2$ conversion to methanol while reducing energy demand. By relying exclusively on simulation-based analysis, this work offers a cost-effective alternative to experimental trial-and-error approaches and supports the development of economically viable $CO_2$ utilisation processes. Overall, this study contributes to sustainable methanol production through kinetic modelling and reaction optimization.

**Model-induced uncertainties of complex turbulent flows in a 3D diffuser**

Hintz, Johanna (1); Mandler, Hannes (1); Kempf, Daniel (2); Weigand, Bernhard (1); Beck, Andrea (1)

*1: University of Stuttgart*
*2: University of Stuttgart (formerly)*

10:10

Turbulent diffuser flows which occur in many technical applications like gas turbine engines or vehicle aerodynamics can suffer from severe total pressure losses. The locations of the separation and reattachment lines are strongly affected by the lateral momentum transport due to the turbulent fluctuations themselves and, in rectangular diffusers, the Reynolds stress anisotropy-driven mean flow vortices. The choice how the turbulence is accounted for in numerical simulations can therefore have a significant effect on their predictive accuracy.

In this study, we quantify this effect and break it down to the influence by (1) the percentage of the resolved turbulent scales, (2) the structure, and (3) the parametrization of the closure model for the unresolved scales. To this end, we performed DNS, LES, and RANS simulations with conceptually different closure models for the ERCOFTAC UFR 4-16 test case [1] (the "Stanford" diffuser).

The considered RANS closures span linear and nonlinear eddy-viscosity models (EVMs) with and without elliptic blending. LESs were performed without an explicit subgrid-scale model and using static as well as dynamic EVMs. Importantly, all DNSs and LESs were performed using the same numerical schemes. The same applies among the RANS simulations.

We find that within the class of RANS closures, the model structure has a larger influence on the predictive accuracy of the mean flow field than its parametrization. A qualitatively correct prediction of the velocity field requires at least a quadratic constitutive law. Unexpectedly, linear EVMs yield more accurate predictions of the total pressure loss than their nonlinear counterparts, which must obviously be a result of cancellation of different modeling errors.

Compared to the implicit closure, the LES results show that a more complex model structure which accounts for the diverse flow field characteristics is more suitable to predict the total pressure loss. Simpler turbulence models, e.g. not capable of computing the correct near wall behavior, can however be improved. This is achieved by dynamically computing the model coefficient. Still, the inherently more sophisticated static models provide a significantly better approximation.

Finally, we will compare the RANS and LES approaches. Here, we will discuss the trade-off between a potential gain in accuracy and the associated increase of the computational costs.

[1] Cherry EM, Elkins CJ, Eaton JK. Geometric sensitivity of three-dimensional separated flows. Int J Heat Fluid Flow 2008; 29(3):803–11.

## S11: Interfacial flows

Organizer(s): von Kameke, Alexandra *(HAW Hamburg)*
Schlüter, Michael *(Hamburg University of Technology)*
Weiland, Christian *(Hamburg University of Technology)*

## S11.01: Modeling Interphase Phenomena

Date: March 18, 2026 16:30–18:30
Room: KII, M17.15
Chair(s): Schlüter, Michael
von Kameke, Alexandra

### Sharp-Interface modeling and numerical simulation of wetting processes

Bothe, Dieter; Fricke, Mathis; Maric, Tomislav 16:30
*TU Darmstadt, Germany*

Mathematical modeling and numerical simulation of wetting processes demand predictive and thermodynamically consistent models as well as accurate and efficient numerical methods that avoid case-specific parameter tuning. The present talk surveys the sharp-interface modeling of two-phase flows with moving contact lines.

Wetting refers to dynamic processes in which portions of the surface of a solid support are freshly covered by liquid molecules, forming the boundary of a bulk liquid portion. In such processes, the contact line around which molecules of all three bulk phases are present, is moving relative to the solid. For a material contact line this can only happen if the liquid slips on the support, at least close to the contact line. However, from a mathematical analysis of the kinematics of the flow near the contact line it can be shown that regular solutions of the two-phase incompressible Navier-Stokes equations with a contact angle relation of type are unphysical for the standard Navier slip boundary condition [1]. This shows the core relevance of appropriate boundary and contact line conditions for a sound modelling of wetting processes. Starting from more classical approaches, we report on most recent developments to capture the contact line dynamics in a thermodynamically consistent manner [2].

On the numerical side, we report on core building blocks needed for direct numerical simulations building on current sharp-interface two-phase numerical approaches based on the Finite Volume method. Special emphasis will be on recent developments achieved within the Collaborative Research Centre 1194 at TU Darmstadt, both concerning numerical method improvements [3, 4] and regarding the development of numerical benchmark cases [5].

**References**

1. M. Fricke, M. Köhne, D. Bothe: A kinematic evolution equation for the dynamic contact angle and some consequences. Physica D **394**, 26-43 (2019).

2. T. Fullana, Y. Kulkarni, M. Fricke, S. Popinet, S. Afkhami, D. Bothe, S. Zaleski: A consistent treatment of dynamic contact angles in the sharp-interface framework via the generalized Navier boundary condition. arXiv: 2411.10762.

3. M. Fricke, T. Maric, D. Bothe: Contact line advection using the geometrical Volume-of-Fluid method, J. Comp. Phys. **407**:109221 (2020).

4. M. H. Asghar, M. Fricke, D. Bothe, T. Marić: Numerical wetting simulations using the plicRDF-isoAdvector unstructured Volume-of-Fluid (VOF) method. Computers & Mathematics with Applications **180**, 191-213 (2025).

5. D. Gründing, M. Smuda, T. Antritter, M. Fricke, D. Rettenmaier, F. Kummer, P. Stephan, H. Marschall, D. Bothe: A comparative study of transient capillary rise using direct numerical simulations, Applied Mathematical Modelling **86**, 142-165 (2020).

**Advanced sub-grid scale modelling applied to bubble phase change problems**

OUALI, Anthony (1,2); MABROUK, Majdi (1); LEMONNIER, Stéphane (1); LALANNE, Benjamin (2); ABBAS, Micheline (2)

*1: DES, ISEC, DPME, L3PI, Univ. Montpellier, CEA Marcoule, France*
*2: Laboratoire de Génie Chimique, Univ. Toulouse, CNRS, INPT, UPS, Toulouse, France*

17:10

Steam bubble evaporation or condensation are numerically challenging phenomena. Two main approaches exist to model such phase-change problems. The first one, Direct Numerical Simulations (DNS), consists in capturing the correct temperature gradient at the interface in order to evaluate the exact phase-change source term. Numerical results of this method can be accurate and predictive, with however, an increasing computational cost with the Jakob number (Ja), which is a dimensionless parameter that compares the amount of energy available in the liquid over the energy absorbed by phase change (latent heat). The second approach uses macroscopic models to estimate the source term without resolving the interface gradient, allowing the study of larger systems at high Ja, but requiring calibration against experiments or theory.

In this work, a sub-grid phase-change model (SGM) is developed, based on the work of Weiner and Bothe [1] for mass transfer problems, with the objective to compute thermal gradients by using coarse mesh grids. The analytical solution of a model problem is used, and fitted in each cell containing an interface, based on an energy balance. The thermal boundary-layer thickness is the free parameter to be determined. The integral of the analytical solution can be computed analytically, assuming a cubic cell. The phase-change source term and the thermal diffusion flux are evaluated from the analytical derivative of the temperature profile. To avoid time-step restrictions, a heat-distribution strategy is employed.

The SGM model has been developed in the TwoPhaseFlow OpenFoam framework [2], and validated in the case of a steam-bubble growing in a superheated liquid (boiling problem). In the absence of gravity, the temporal evolution of the bubble radius is monitored and compared with the analytical solution of Scriven [3]. Results are compared with DNS for various Jakob numbers between Ja=3 and 30. The ability of the model to converge correctly with the mesh is demonstrated. As the Jacob number increases, the robustness of the SGM improves compared to the DNS approach.

[1] A. Weiner et D. Bothe, « Advanced subgrid-scale modeling for convection-dominated species transport at fluid interfaces with application to mass transfer from rising bubbles », *Journal of Computational Physics*, **2017**

[2] H. Scheufler et J. Roenby, « TwoPhaseFlow: A Framework for Developing Two Phase Flow Solvers in OpenFOAM », *OpenFOAM® Journal*, **2023**

[3] L. E. Scriven, « On the dynamics of phase growth », *Chemical Engineering Science*, **1959**

**Arbitrary Lagrangian-Eulerian surface discretizations for self-evolving Navier-Stokes manifolds**

Sauer, Roger A. (1,2)

*1: Ruhr University Bochum, Germany*
*2: Gdansk University of Technology, Poland*

17:30

This work presents a new arbitrary Lagrangian-Eulerian (ALE) surface theory and corresponding finite element implementation for area-incompressible Navier-Stokes flow on self-evolving manifolds [1,2]. The formulation is physically frame-invariant, applicable to large deformations, and relevant to fluidic surfaces such as soap films, capillary menisci and lipid membranes. Its unknowns are the fluid velocity, fluid pressure and surface mesh motion. The resulting three-field system is monolithically coupled, and fully linearized within the Newton-Rhapson solution method. It is implemented in a nonlinear surface finite element framework using the pressure stabilization scheme of [3] and the mesh stabilization scheme of [4], which are all adapted here to the new ALE frame. The unknown ALE mesh motion is determined by membrane elasticity such that the in-plane mesh motion is stabilized without affecting the physical behavior of the system. The new formulation is demonstrated on

several challenging examples including shear flow on self-evolving surfaces, and inflating soap bubbles with partial inflow on evolving boundaries. Optimal convergence rates are obtained in all cases. Particularly advantageous are C1-continuous surface discretizations, for example based on NURBS.

[1] R.A. Sauer (2025), A curvilinear surface ALE formulation for self-evolving Navier-Stokes manifolds – General theory and analytical solutions, J. Fluid Mech., 1016:A34
[2] R.A. Sauer (2025), A curvilinear surface ALE formulation for self-evolving Navier-Stokes manifolds – Stabilized finite element formulation, Comput. Methods Appl. Mech. Engrg., 447:118331
[3] C.R. Dohrmann and P.B. Bochev (2004), A stabilized finite element method for the Stokes problem based on polynomial pressure projections, Int. J. Numer. Methods Fluids, 46:183-201
[4] R.A. Sauer (2014), Stabilized finite element formulations for liquid membranes and their application to droplet contact, Int. J. Numer. Meth. Fluids, 75(7):519-545

**Computational Design of Mesh Structures for Enhanced Interface Stability Using a Phase-Field Method**

Wagner, Alexander; Bonart, Henning 17:50
*Technische Universität Darmstadt, Fachbereich Maschinenbau, Germany*

Wetting of structured meshes is essential for many process engineering applications, including gas diffusion electrodes (GDEs) in electrochemistry, where a gas-liquid interface forms inside a structured electrode, separating the liquid electrolyte and the gaseous reactant. Stability of the gas-liquid interface is crucial but particularly challenging in organic electrosynthesis, where small contact angles promote electrode flooding and performance loss. Here, we investigate strategies to stabilize the gas-liquid interface by imposing a specifically controlled pressure difference in combination with tailored mesh structures. To quantify admissible Laplace pressures and explore the mesh design, we employ numerical phase-field simulations based on the coupled Cahn-Hilliard-Navier-Stokes equations implemented in OpenFOAM. We first analyze wetting behavior and bubble growth at single, differently shaped orifices and demonstrate the significant influence of the orifice geometry on the differential pressure range over which stable phase separation can be maintained. Building on these results, we investigate more complex mesh structures with varying geometries and surface wettabilities, requiring large-scale simulations performed on high-performance computing systems. In addition, we examine the effects of crossflow and pulsating conditions on the stability of the gas-liquid interface. From our findings, we derive design guidelines for mesh structures that enhance interface stability. These guidelines enable the design of improved GDE architectures, supporting their reliable application in organic electrosynthesis and facilitating scale-up toward industrial applications.

**Pore-scale evaporation dynamics: Microfluidic experiment and pore-network modelling**

Veyskarami, Maziar (1); Raoof, Amir (2); Helmig, Rainer (1) 18:10
*1: Universität Stuttgart, Germany*
*2: Utrecht University, Netherlands*

The processes occurring at the pore scale and their link to macroscopic system behavior can reveal key mechanisms that govern overall transport and reaction in porous media. Microfluidic experiments are a powerful tool that enables direct observation of pore-scale phenomena with high spatial and temporal resolution (Mourab et al. 2019). Pore-network modeling, which represents interactions that are typically homogenized in continuum-scale models, complements these experiments and provides deeper insight into the underlying pore-scale behavior (Weishaupt & Helmig, 2021).

Accurately representing the coupled evolution of liquid films, interface curvature, and evaporation kinetics in complex porous structures remains a central difficulty for predictive models. To address this, high-resolution microfluidic measurements are integrated with dynamic pore-network modeling, yielding time-resolved data on water configurations, saturation, and curvature, alongside a mechanistic interpretation of the controlling pore-scale processes. Our integrated model-experiment analysis elucidates how critical pore-scale processes—such as competitive evaporation and corner flow of the wetting phase—govern evaporation dynamics within microfluidic porous media.

This study seeks to deepen the understanding of pore-scale evaporation dynamics. Systematic comparison between experimental observations and simulation outputs, combined with a detailed analysis of their discrepancies, reveals experiment-specific features that are not fully represented in the model and clarifies the inherent uncertainties associated with microfluidic measurements. The results show that these uncertainties can strongly influence both the apparent quality of agreement and the conclusions drawn from model validation, making benchmarking of pore-scale models inherently challenging.

References:

Weishaupt, K., & Helmig, R. (2021). A Dynamic and Fully Implicit Non-Isothermal, Two-Phase, Two-Component Pore-Network Model Coupled to Single-Phase Free Flow for the Pore-Scale Description of Evaporation Processes. *Water Resources Research*, *57*(4). https://doi.org/10.1029/2020wr028772

Moura, M., Flekkøy, E. G., Måløy, K. J., Schäfer, G. & Toussaint, R. (2019). Connectivity enhancement due to film flow in porous media. Physical Review Fluids, 4(9), 094102. https://doi.org/10.1103/PhysRevFluids.4.094102

## S11.02: Particles & Mixing

Date: March 19, 2026 08:30–10:30
Room: KII, M17.15
Chair(s): Weiland, Christian
von Kameke, Alexandra

### Solving the Maxey-Riley-Gatignol equations: simulation, analysis and tracking of inertial particles

Rathi, Vamika (1); Sommer, Finn (1); Sehar, Fatima (1); Urizarna-Carasa, Julio (1); Goetschel, Sebastian (1); Steuwe, Eike (2); von Kameke, Alexandra (2); Padberg-Gehle, Kathrin (3); Ruprecht, Daniel (1)

*1: Hamburg University of Technology*
*2: Hamburg University of Applied Sciences*
*3: Leuphana University Lüneburg*

08:30

Particles moving within a fluid are a ubiquitous phenomenon, appearing in contexts ranging from virus-laden saliva droplets suspended in air, to plankton sedimentation in the ocean, to particles in high-pressure jets during oxy-coal combustion, and Lagrangian sensors collecting data within the fluid. While very small particles tend to follow the flow passively, larger particles experience additional forces such as drag and wake effects. Although fully resolved fluid-structure interaction (FSI) simulations can capture the detailed interactions at the fluid-particle interface, these models are computationally intensive, often requiring days or weeks of runtime. Consequently, they are invaluable for fundamental research but impractical for applications demanding near real-time analysis.
The Maxey-Riley-Gatignol equations (MaRGE) offer a significantly simplified model for spherical particles of moderate size moving without collisions. MaRGE accounts for Stokes drag as well as history-dependent wake effects, whereby the forces acting on a particle depend on its past trajectory. Mathematically, the history term appears as an integral in the governing equations, posing a challenge for efficient numerical solution. As a result, this term is frequently neglected, despite its potential qualitative and quantitative significance in many scenarios.
In this presentation, we compare three numerical methods for solving MaRGE and demonstrate that, unlike full FSI models, they can achieve errors below 1% while operating in near real-time. Since individual trajectories may not always be the primary focus, we further analyze clustering patterns and finite-time Lyapunov exponents, highlighting that the history term also has a non-negligible influence on the larger-scale dynamics of inertial particles. Finally, we propose a framework for employing MaRGE as a dynamic model in filtering algorithms aimed at tracking Lagrangian sensors in a stirred tank reactor. Using synthetic measurements from an inertial measurement unit (IMU), we compare the performance of an extended Kalman filter and a particle filter for tracking particles in the realistic flow field of a lab-scale stirred reactor.

**Dynamical compartments in stirred tank reactors and Markov state modeling for mixing quantification**

Thai, Thanh Tung (1); Steuwe, Eike (2); Klünker, Anna (1); Weiland, Christian (3); von Kameke, Alexandra (2); Padberg-Gehle, Kathrin (1)

*1: Leuphana University Lüneburg, Germany*
*2: HAW Hamburg, Germany*
*3: Hamburg University of Technology, Germany*

09:10

Analyzing fluid transport and mixing in chemical reactors is crucial to find and avoid dead zones and control concentration distributions. Recent computational methods can identify these finite-time coherent sets directly from fluid particle trajectories obtained from numerical simulations or laboratory experiments, such as particle tracking (4D-PTV).
This contribution demonstrates the application of trajectory-based approaches of identify coherent flow structures in chemical reactors and analyze their transport properties. In particular, we consider a spectral clustering framework for the approximation of coherent sets that form dynamical compartments in a stirred tank reactor. We propose methodological extensions that allow us to study global transport and mixing by means of a Markov state model, with these compartments being the Markov states. The proposed computational approaches have been implemented in Python to improve performance, accessibility and versatility.

**Modeling and simulation of CMAS particle interaction with hot turbine surfaces**

Selvaraj, Ravishankar (1); Vogel, Andreas (2); Oevermann, Michael (1)

*1: Brandenburg University of Technology, Germany*
*2: Rolls-Royce Deutschland Ltd & Co KG*

09:30

Aircrafts operating in dusty environments such as deserts or regions affected by volcanic activity are susceptible to ingesting fine mineral dust and volcanic ash into their engines. Once entrained in the hot gas path, these particles may soften or melt before impacting hot turbine components, including guide vanes and blades. Depending on their thermophysical state and impact conditions, molten ash particles can bounce, adhere, or splash upon contact. Over-extended operation times under such conditions deposit layers might develop, which partially obstruct airflow, degrade compressor and turbine efficiency, and increase the risk of engine surge. These effects significantly compromise engine performance, durability and maintenance requirements.

To achieve a quantitative understanding of molten ash particle dynamics, a comprehensive numerical modelling framework is developed to capture particle transport, impact, and deposition on both static and rotating turbine surfaces. The methodology employs an Euler–Lagrangian computational fluid dynamics (CFD) formulation, in which the carrier gas phase is solved using an Eulerian approach while dispersed mineral particles are tracked in a Lagrangian framework. Constitutive models for Calcium–Magnesium–Aluminium–Silicate (CMAS) particles are incorporated to represent temperature-dependent thermophysical properties, including melting behaviour and viscosity, using polynomial-based correlations.

Particle-wall interactions are here predicted using a sticking probability model that couples a critical-viscosity criterion with a coefficient-of-restitution formulation. The model incorporates particle temperature, viscosity, impact velocity and angle, and collision energy dissipation to distinguish between sticking and rebound regimes. In contrast to the assumption of rigid particles, the developed model also accounts for particle deformation by incorporating elasto-plastic impact regimes, allowing a more realistic representation of molten and semi-molten ash behaviour. Based on the Tafti sticking model [1][2], the formulation is implemented and extended within an OpenFOAM simulation framework to improve robustness and predictive accuracy under engine-relevant operating conditions.

We show results for capture efficiency and impact efficiency as a function of temperature, along with comparisons to experimental data. The resulting modelling capability enables reliable estimation of ash deposition rates and supports the design, certification, and operation of high-performance turbine engines.

1. Sukhjinder Singh, Danesh Tafti, Particle deposition model for particulate flows at high temperatures in gas turbine components, International Journal of Heat and Fluid Flow, Volume 52, 2015, Pages 72-83, ISSN 0142-727X, http://doi.org/10.1016/j.ijheatfluidflow.2014.11.008

2. Sai Shrinivas Sreedharan, Danesh K. Tafti, Composition dependent model for the prediction of syngas ash deposition in turbine gas hotpath, International Journal of Heat and Fluid Flow, Volume 32, Issue 1, 2011, Pages 201-211, ISSN 0142-727X, http://doi.org/10.1016/j.ijheatfluidflow.2010.10.006

**Reduction-consistent thermodynamic modeling and computation of compressible and incompressible N-phase mixture flows**

ten Eikelder, Marco; Schillinger, Dominik 09:50
*TU Darmstadt, Germany*

Modern simulation and modeling approaches for multiphase mixture systems face substantial challenges. These challenges extend beyond computational complexity, reflecting a deeper issue: the absence of a standardized mathematical framework. As a result, existing models struggle to accurately capture the full intricate dynamics of multiphase mixtures, and the connection between various modeling approaches remains unclear.
In this presentation, we introduce a unified modeling and computational framework tailored for both compressible and incompressible N-phase mixture flows. Rooted in continuum mixture theory, this framework derives governing equations and phase-field closure models from first principles.
We develop a reduction-consistent thermodynamic closure for N-phase mixture models and a practical calibration procedure for prescribed pairwise surface tensions.
This provides a versatile hierarchy of models, ranging from comprehensive systems of balance laws to simplified yet physically consistent formulations. We analyze this framework by comparing it with existing models through both theoretical and computational perspectives. Finally, we discuss structure-preserving finite element methods and demonstrate their application to benchmark problems in N-phase flow simulations.

**Numerische Analyse der Zweiphasenströmung und der Wärmeübertragung in geschlossenen Thermosiphon-Sonden**

Wang, Qiaoleiyue; Brenner, Gunther 10:10
*TU Clausthal, Germany*

Geschlossene Zweiphasen-Thermosiphon-Sonden sind eine innovative Lösung im Bereich der Geothermie, da sie ohne Hilfsaggregate wie Pumpen auskommen. Das Arbeitsmedium, beispielsweise Kohlendioxid, zirkuliert aufgrund der Schwerkraft und der Dichteunterschiede der beiden Phasen in der geschlossenen Sonde. An der Innenwand bildet sich aufgrund des Phasenwechsels ein Flüssigkeitsfilm aus. Die Wärmeübertragungsleistung der Sonde hängt wesentlich von der Dynamik des Flüssigkeitsfilms (Filmdicke, Welligkeit etc.) ab. Daher ist die Untersuchung dieser Strömung für die Optimierung des Betriebsverhaltens der Sonde von großer Bedeutung.

In der vorliegenden Arbeit wird die Strömung sowie die konjugierte Wärmeübertragung in der Sonde und der Formation mittels numerischer Simulation (CFD) analysiert. Die Auflösung der extrem dünnen Flüssigkeitsfilme im Bereich zehntel-Millimeter mit einem drei-dimensionalen numerischen Gitter stellt dabei eine besondere Herausforderung dar. Daher wird in der vorliegenden Arbeit stattdessen ein 2D-Filmmodell, das in OpenFOAM implementiert ist, verwendet, um die Ausbreitung des Films über größere Bereich des Innenrohrs effizient berechnen zu können. Das Modell basiert auf den Flachwassergleichungen und Transportgleichungen für Energie. Damit lassen sich die zeitliche und räumliche (in 2D) Entwicklung der Filmdicke, die wandparallele Filmgeschwindigkeit und die mittlere Filmtemperatur bzw. der Wärmeübergang berechnen. Die Temperatur in der Formation um

die Sonde sowie die gasförmige Strömung im Innern des Rohrs werden durch entsprechende dreidimensionalen Modelle beschrieben. Zur Verifizierung des Modells werden die Nusselt'sche Wasserhauttheorie und die analytische Lösung der Wärmeleitung herangezogen. Zudem wird eine Parameteruntersuchung durchgeführt, um verschiedene Szenarien des lokalen Betriebszustands der Sonde zu simulieren. Das Ziel besteht darin, eine optimierte Auslegung und einen verbesserten Betrieb der Sonde zu ermöglichen und somit das Potenzial der Geothermie maximal auszuschöpfen.

## S11.03: Multiphase Heat and Mass Transfer

Date: March 19, 2026 14:00–16:00
Room: KII, M17.15
Chair(s): von Kameke, Alexandra
Schlüter, Michael

### When hydrogen bubbles break our models

Baltussen, Maike; van den Eertwegh, Danny; Kuipers, Hans 14:00
*Eindhoven University of Technology*

In alkaline water electrolysis, the gas bubble formation, especially the hydrogen bubbles, limits the performance of the electrolysis cell. A detailed understanding of the nucleation, growth and detachment of the bubbles near the electrode will allow further optimization of electrolyzer design and operation, and ultimately for improving the competitiveness of green hydrogen.

Due to the relatively small bubble size and the dense bubble swarms formed near the electrode, experimental studies are generally limited to idealized conditions, for example the experiments are performed under limited current densities or microelectrode setups. Under these conditions, bubble-bubble interactions are limited, despite their importance under realistic operating conditions.

As a result, modelling approaches are required to gain more understanding of the hydrogen formation in realistic conditions. While this may appear straightforward, hydrogen bubbles pose significant challenges to the state-of-the art gas-liquid interface models. For example, their small bubble size results in a high surface tension and consequently a high pressure jump over the surface. In many gas-liquid methods, these high pressure jumps cause strong parasitic currents, which hinder or even prevent the simulation of realistic conditions.

### Experimental Characterization of Two-Phase Flow Regimes in Optically Accessible Fuel-Cell Cathode Plates

Lehle, Moritz; Homner, Sebastian; Stroh, Alexander; Frohnapfel, Bettina; Kriegseis, Jochen 14:40
*Karlsruher Institut für Technologie (KIT), Germany*

Fuel cells are a key technology for the transformation of the energy sector. They enable the direct conversion of hydrogen into electrical power, bypassing combustion and the associated pollution. A major limitation to their performance and durability comes from liquid-water formation in the cathode-side microchannels. This accumulated liquid can partially or fully block the flow passages and locally inhibit electrochemical activity. Depending on the given flow conditions, the resulting two-phase flow leads to different flow regimes. To improve the efficiency of fuel-cell systems, a deeper understanding of the flow dynamics of the forming regimes is necessary.
In this work, an experimental approach is developed that provides direct optical access to the parallel microchannels of a cathode plate, while preserving the relevant physical boundary conditions for an in-situ operation. Transparent window materials were evaluated with respect to their wetting behavior in comparison to the cathode plate. Such matching pairs are essential to ensure that observed flow phenomena are representative of realistic in-situ operating conditions.
The functionality of the optically accessible plate was demonstrated in a series of ex-situ experiments with a controlled-air and superheated-steam supply to minimize the complexity of setups for in-situ operation of fuel cells. High-speed reflected-light shadowgraphy measurements were carried out to resolve the spatio-temporal evolution of the two-phase flow within the microchannels. The detection of flow regimes in the image data is greatly influenced by the small dimensions of the channels. In

addition to small-scale channels, complex backgrounds caused by fibrous gas diffusion layers play a role, making evaluation routines even more difficult. This poses significant challenges for conventional image-based flow regime classification.
Recurrence plots derived from time-resolved image data capture the intrinsic temporal structure of the flow and reveal characteristic patterns associated with different flow regimes. This approach enables an easy, fast and reproducible identification of regimes and moreover transitions without relying on manual and subjective visual classification with conventional image-processing methods.
Overall, the presented methodology combines tailored optical access, wetting and interfacial analysis with data-driven time-series evaluation to provide a comprehensive framework for the investigation of two-phase flow regimes in fuel-cell-relevant microchannels.

**A Lagrangian Analysis of the Depletion of Substrates in the Gaseous Phase and the Effect on Mass Transfer**

Weiland, Christian (1); Rogel, Madlen (1); Steuwe, Eike (2); Thai, Thanh Tung (3); Klünker, Anna (3); Padberg-Gehle, Kathrin (3); von Kameke, Alexandra (2)
*1: Hamburg University of Technology, Germany*
*2: HAW Hamburg, Germany*
*3: Leuphana University Lüneburg, Germany*

15:00

In the course of the Collaborative Research Centre 1615 "SMART Reactors for Future Process Engineering", funded by the German Research Foundation, new reactor types are developed to face climate change.

Since many relevant processes include multiphase phenomena, a precise estimation of the coupled mass transfer might be of crucial interest. The current work focusses on this and investigates the performance of aerated stirred tank reactors numerically. Hereby, the occurring gas bubbles are observed individually along their respective path through the vessel. They are allowed to experience coalescence and breakup events. The latter is described by the Trajectory-Based Breakup Model [1,2]. For the quantification of the mass transfer, the surface areas of the individual bubbles are taken into account together with the local concentration differences and interfacial or boundary layer conditions, yielding individual mass transfer coefficients for each bubble which might change in the course of time. Examined will be two different species: one will be transferred from the bubble into the liquid. This is often a substrate which is necessary for a consecutively following liquid phase reaction. The other one will be transferred from the liquid into the bubble. This is mirroring either a by-product yielding from the reaction, like carbon dioxide in fermentation processes, which has the potential to inhibit the reaction or another gaseous component which might be left behind from a preceding stripping process like nitrogen. Altogether, both mass transfer processes have the potential to deplete the concentration of the substrate in the gas bubbles, which consequently leads to a less efficient process due to lowering the local concentration difference. The effect of the depletion on the mass transfer efficiency is examined and quantified for each bubble along its respective trajectory.

[1] Weiland, C.; von Kameke, A.; Schlüter, M. (2024). Trajectory-based breakup modelling for dense bubbly flows. Chemical Engineering Journal. 499. 155726.

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**Approach towards Pulsating Heat Pipe Performance Prediction using Gradient Boosting and Experimental Iteration**

Franke, Friedrich (1); Illbruck, Marvin (1); Kober, Markus (1); Enghardt, Lars (1,2); Kazula, Stefan (1)
*1: Deutsches Zentrum für Luft- und Raumfahrt, (German Aerospace Center), Germany*
*2: Brandenburgische Technische Universität Cottbus - Senftenberg*

15:20

Pulsating heat pipes (PHPs) are compact, two-phase heat transfer devices that have attracted substantial research interest across various engineering fields. Their high equivalent thermal conductivity make them particularly promising for applications requiring high heat transfer under stringent space constraints, such as aviation or space systems.

PHPs consist of capillary channels which are bent into multiple conjoined U-turns called meanders that are often connected to form one continuous loop. These channels are filled with a working fluid, where a part of the fluid is in the liquid and part of it is in the vapor state. Due to the small diameter of the channels, the capillary forces acting upon the fluid arrange the two phases into an intermittent pattern of liquid slugs and vapour bubbles.

During operation thermal energy is transferred in the device through a complex interaction of fluid dynamic phenomena. Vapor plugs expand and contract, leaving behind evaporating liquid films, nucleate boiling leads to the formation of new bubbles and moving liquid slugs compress adjacent gas bubbles resulting in self-sustained pulsating oscillations, from which the name of the device is derived. A lot of research has been conducted on the working principle of PHPs and many avenues of predicting thermal performance have been implemented.

However, detailed simulations of the internal fluid dynamics are very costly, take up a large amount of time, do not produce reliable results for thermal performance and lack the capability to predict performance of new configurations.

This work introduces a Methodology to interpret and predict PHP performance data. An extreme gradient boosting (XGB) algorithm is trained with datasets from literature and experiments. XGB employs parallelized tree-building and use of gradient descent with regularized Newton–Raphson to prevent overfitting. A game-theory based interpretation method is applied to evaluate the impact of features on the models prediction across the datasets.
In addition, an experimental framework is developed to quantify the impact of various PHP features and investigate novel PHP configurations as well as their influence on thermal performance. A high vacuum PHP filling rig and a thermal conductivity measurement setup are tested and put into operation with a focus on quick geometric PHP iteration.

The combined application of data interpretation and experimentation offers an efficient approach for PHP performance estimation with reduced resource requirements, facilitating the rapid development of PHPs for various applications.

**Numerical simulations of interfacial mass transfer around rising bubbles contaminated by soluble surfactants**

Kentheswaran, Kalyani (1,2,3); Dietrich, Nicolas (2,3); Lalanne, Benjamin (1,3) 15:40
*1: University of Toulouse, France / Chemical Engineering Lab*
*2: University of Toulouse, France / Toulouse Biotechnology Institute*
*3: FERMaT*

Accurate prediction of interfacial mass transfer in bubbly flows is crucial for the optimization of many (bio-)chemical processes. In the presence of amphiphilic species such as surfactants, colloidal particles, or alcohol, strong modifications of bubble hydrodynamics are observed due to adsorption at the interface, surface tension gradients and resulting Marangoni stresses. Experiments consistently report a significant decrease of mass transfer rates around contaminated bubbles, but its origin is still debated: it may arise from changes in bubble hydrodynamics (Marangoni stresses) or from an intrinsic hindrance confered by the adsorbed species. In this work, we use Direct Numerical Simulations to simulate mass transfer around rising bubbles in the presence of soluble surfactants. The objective is to develop physical models able to predict the decrease of the Sherwood number solely due to Marangoni stresses. Simulations are performed with the in-house code DIVA, based on the Level-Set and Ghost Fluid methods. Surfactant transport is solved both in the bulk and along the interface, including adsorption–desorption fluxes described by Langmuir kinetics. Surface tension locally varies, leading to Marangoni forces which are coupled to the Navier–Stokes equations. Gas–liquid mass transfer is computed through an advection–diffusion equation, by assuming liquid-side resistance.

Two hydrodynamic regimes are investigated: the stagnant-cap (SC) and uniformly retarded (UR) regimes, which depend on the relative time scales of (i) surfactant exchange between the bulk and the interface and (ii) surface transport. The SC regime exhibits a clear contamination angle for the bubble, separating a mobile and immobile region, while in the UR regime the interface remains partially mobile everywhere. The intensity of the Marangoni stresses is indeed measured to be smaller in

the UR regime, at same coverage rate. In both cases, the Sherwood number lies between the clean-bubble and rigid-sphere limits. A local analysis shows that mass transfer is mainly controlled by the hydrodynamics near the bubble front, and occurs at a smaller rate than for a clean bubble at same Reynolds Re and Schmidt Sc numbers. The decline in the interface mobility, as compared to a bubble not submitted to Marangoni stresses, is found to be mostly responsible for that. A dimensionless parameter based on the maximum tangential velocity is introduced to quantify this effect. Using it, a general correlation for the Sherwood number of contaminated bubbles is proposed, valid over 1 $\leq$Re $\leq$100, 1 $\leq$Sc $\leq$500, for both the SC and UR regimes.

## S11.04: Multiscale Interfacial Flows

Date: March 20, 2026 08:30–10:30
Room: KII, M17.15
Chair(s): Weiland, Christian
von Kameke, Alexandra
Schlüter, Michael

### A minimalist model for the capture and investigation of solitary waves in gravity-driven liquid films

Scholle, Markus (1); Al Ahmadi Hammou, Meriem (2); Gaskell, Philip H. (3)
*1: Heilbronn University, Germany*
*2: Heilbronn University, Germany*
*3: Durham University, UK*

08:30

A potential-based, first-integral formulation of the Navier-Stokes equations is used as the platform for modelling solitary waves in the context of gravity-driven film flow on planar surfaces, resulting in a nonlinear partial differential equation (PDE), in complex form.
Its subsequent modal decomposition, leading to an infinite set of ordinary differential equations (ODEs), followed by a bimodal approximation and elimination of unknowns, results in just two coupled ODEs to be solved. The latter is achieved both analytically and numerically using a Ritz-Galerkin methodology. Illustrative solitary wave results are provided, which exhibit the expected internal recirculating flow pattern and the corresponding pronounced hump-shaped, free-surface displacement typically observed in related experiments and consistent with other analytical/numerical results in the literature. Despite the numerous approximations involved in arriving at such a minimalist model, the same is capable of providing valid predictions apropos solitary waves; namely, regarding the existence of multiple solutions for a given film thickness and effective inclination angle, with different size and propagation speed, as demonstrated by the parameter study undertaken. Another remarkable feature is the paired occurrence of solitary wave and anti-wave solutions.

### Analytical Modelling of Capillary-Driven Heat Transfer in Micro Heat Pipe

Singh, Manjinder
*Malaviya National Institute of Technology Jaipur, India*

08:50

Micro heat pipes (MHPs) provide an effective passive approach for dissipating heat from microelectronic devices by exploiting phase-change processes. A typical MHP comprises a sharp-edged microchannel filled with a working fluid. Capillary action along the sharp edges drives the liquid flow, while vapor travels through the central core of the channel. Axially, the heat pipe is divided into three regions: the evaporator, adiabatic, and condenser sections.

In this study, an analytical mathematical model is developed to describe heat transfer in a micro heat pipe. The model is solved as a function of the liquid–vapor interface radius of curvature and the solid–liquid contact angle to predict the maximum steady-state heat transfer rate. The maximum heat transport capacity of an MHP is reached when the evaporator section becomes dry. At any axial location, the amount of liquid present depends on the local liquid cross-sectional area, which is governed by the radius of curvature of the liquid–vapor interface.

The axial variation of the interface curvature is obtained by relating it to the pressure difference across the liquid–vapor interface using the Young–Laplace equation, , where is the surface tension. Differentiating this relation with respect to the axial coordinate yields a differential equation describing the axial evolution of the interface curvature. Uniform heat input in the evaporator and uniform heat removal in the condenser are assumed, along with an axially uniform vapor pressure. The resulting equation is integrated separately for each section, with integration constants determined by using the interface curvature at the end of one section as the boundary condition for the next.

The analysis shows that the radius of curvature increases monotonically from the evaporator to the condenser. This behaviour arises because heat addition in the evaporator promotes evaporation, causing the liquid–vapor interface to recede into the groove corners and reducing the radius of curvature. Conversely, heat removal in the condenser leads to vapor condensation and liquid accumulation, advancing the interface and increasing its curvature. This monotonic increase in curvature generates a Laplace pressure gradient within the liquid, which drives liquid flow from the condenser back to the evaporator.

**Map-based modeling of intermittency effects on coagulation of zero-inertia particles in inertial-range turbulence**

Medina Méndez, Juan A. (1); Starick, Tommy (1); Klein, Marten (1); Schmidt, Heiko (1); Kerstein, Alan R. (2) 09:10

*1: Numerische Strömungs- und Gasdynamik, BTU Cottbus-Senftenberg, Germany*
*2: Independent Consultant, USA*

The time evolution of a population of zero-inertia particles in a turbulent flow, distributed within a one-dimensional (1-D) domain, is simulated using a specialization of a map-based particle-collision model, ClusColl [1]. The idealized setup allows a detailed evaluation of the coagulation process under the assumption of sustained inertial-range turbulence. The underlying focus is the relation between Lagrangian particle-correlation statistics and the anomalous inertial-range scaling of the third-order passive-scalar turbulence structure function, leading to temporally-correlated coagulation events [2]. In contrast to standard Smoluchowski kinetics [3], these intermittency effects enhance coagulation rates, and in particular lead to an anomalous scaling with respect to the dimensional prediction [2]. Previous numerically supported analytical work by [4] established that the so-called triplet map used here, as in [1], yields a third-order scalar structure function exponent value close to the physical value, and accordingly, the present numerical results yield particle-size-dependent coagulation-rate exponents in close agreement with those previously reported in [2]. The remarkable fidelity of the present 1-D formulation is enabled by the treatment of particle motion as a jump process [1], rather than a continuous trajectory. In conjunction with [1], this supports the future development of a highly efficient yet physically sound modeling of particle coagulation in inertial-range turbulence.

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**Stability and Instability in Anisotropic Multi-Phase Interface Evolution**

Eto, Tokuhiro (1); Garcke, Harald (2); Nürnberg, Robert (3) 09:30

*1: Université Claude Bernard Lyon 1, CNRS, Centrale Lyon, INSA Lyon, Université Jean Monnet, ICJ UMR5208, 69622 Villeurbanne, France*
*2: Fakultät für Mathematik, Universität Regensburg, 93040 Regensburg, Germany*
*3: Dipartimento di Mathematica, Università di Trento, 38123 Trento, Italy*

*We consider a sharp interface formulation for an anisotropic multi-phase Mullins–*

*Sekerka problem with kinetic undercooling. The flow is characterized by a cluster of surfaces evolving such that the total surface energy plus a weighted sum of the volumes of the enclosed phases is decreased in time. Upon deriving a suitable variational formulation, we introduce a fully discrete unfitted finite element method. That is, the approximations of the moving interfaces are independent of triangulation that is used for the equations in the bulk. Our method can be shown to be unconditionally stable. Several numerical examples demonstrate the capabilities of the introduced method.*

**Virtual One-Dimensional Turbulence (VODT) for Subgrid Primary Breakup in Interfacial Flows**

Munhoz-Boillot, Ionawr; Oevermann, Michael 09:50
*Brandenburgische Technische Universität Cottbus-Senftenberg, Germany*

Primary atomization in shear-driven interfacial flows results from a tight coupling between turbulent eddies, surface tension effects on ligament thinning and pinch-off. While direct numerical simulation can resolve these mechanisms, it remains impractical at Reynolds and Weber numbers typical of flow atomization. In LES simulation with volume-of-fluid (VOF) interface capturing, the smallest interfacial deformations and breakup events fall below the grid scale, which limits predictive capability for droplet production rates, size distributions, and the recession of the resolved liquid core.

Virtual One-Dimensional Turbulence (VODT) provides a reduced-order subgrid description of turbulence–interface interaction that is derived from the one-dimensional turbulence (ODT) framework. The method considers a one-dimensional line locally aligned with the interface normal and prescribes a piecewise-linear velocity profile across liquid and gas that represents the local shear state. Multiphase eddy events are sampled statistically, and their stationary event-rate distribution is used to evaluate breakup statistics without explicitly evolving the full mapped fields. This yields a droplet-size probability density function together with integral measures such as droplet production rate and interface-recession speed, which can be translated into source terms for subgrid mass transfer from resolved liquid to dispersed droplets.

In this work, a robust standalone VODT formulation is established and assessed against high-fidelity reference data. From DNS of primary droplet production on a selected interface segment, we extract the droplet-size distribution, droplet production rate, and recession speed. For the investigated breakup regime, VODT reproduces the DNS-derived statistics with very similar trends and magnitudes, indicating that the reduced stochastic description captures the dominant physics controlling primary droplet generation.

Ongoing work targets the integration of VODT as a subgrid-scale model within LES to predict cell-wise primary droplet creation in VOF simulations and to initialize droplet populations consistently with local resolved flow conditions, with the goal of recovering DNS-consistent atomization metrics at practical computational cost.

## S12: Waves and Acoustics

Organizer(s): Langer, Sabine *(TU Braunschweig, Institut für Akustik und Dynamik)*
Keßler, Manuel *(Universität Stuttgart)*

## S12.01: Waves and Acoustics

Date: March 20, 2026 08:30–10:30
Room: KII, M17.72
Chair(s): Keßler, Manuel
Langer, Sabine

### A time-domain boundary element method for acoustics with generalized convolution quadrature and adaptive fast multipole evaluation

Arora, Nikhil; Schanz, Martin 08:30
*Technical University of Graz, Austria*

The time-domain Boundary Element Method (BEM) for the homogeneous acoustic wave equation with vanishing initial conditions is considered. Spatial discretization is performed using low-order boundary elements, while temporal discretization is based on the generalized Convolution Quadrature (gCQ) method. Within the gCQ framework, the discrete convolution in time requires the evaluation of boundary integral operators in the Laplace domain at several complex frequencies. These matrices are approximated using Chebyshev interpolation based Fast Multipole Method (FMM), such that the computational cost of the convolution is governed by the number of multipole-to-multipole (M2M), multipole-to-local (M2L), and local-to-local (L2L) translations. If a uniform FMM tree is used, the same refinement pattern is applied across the entire boundary, which results in a larger number of M2M, M2L, and L2L translations than necessary. In this work, an adaptive FMM is employed to reduce the number of translation operations required for each operator application while preserving the accuracy of the kernel approximation. In addition, the dependence on the complex frequencies is approximated by selecting only a subset of frequencies along the contour, thereby compressing not only the spatial interactions but also the frequency dimension.

The purpose of this study is to quantify the impact of spatial adaptivity in the FMM on the efficiency of the gCQ-based time-domain BEM in the presence of frequency-domain compression. A systematic comparison between uniform and adaptive FMM is carried out, demonstrating that the reduction in translation operations achieved by adaptivity leads to a significant decrease in the computational cost of the convolution, particularly for geometries with non-uniform distributions. The effectiveness of the proposed approach is illustrated by acoustic scattering problems involving a unit cube and a unit cube with a reentrant corner.

### Time Domain Boundary Element Methods for the Neumann Problem: A Reduced Approach for Practical Applications

Schneider, Simon (1,3); Özdemir, Ceyhun (2); Gimperlein, Heiko (2); Urban, Karsten (1); Graf, Bernd (3) 08:50
*1: Ulm University, Germany*
*2: University of Innsbruck, Austria*
*3: Ulm University of Applied Sciences, Germany*

There is a strong interest in accurately predicting acoustic fields in compliance with relevant standards and regulations. This is one reason why Noise, Vibration, and Harshness (NVH) analyses remain an important aspect of industrial applications and have become recognized as a distinct engineering discipline.
Structure-borne sound can be computed directly in the time-domain using multibody simulations. In contrast, the radiated sound pressure waves are usually determined in the frequency-domain since direct time-domain calculations often face challenges regarding numerical stability and computational cost. Nevertheless, there is a growing interest in predicting sound radiation directly in the

time-domain in order to capture transient phenomena, such as engine start-up or shutdown, acceleration processes, or other events involving a broad frequency spectrum.
Our previous work focuses on a stable Boundary Element Method (BEM) formulation using a hypersingular operator to solve a first-kind integral equation. For sound radiation in large unbounded domains, the BEM offers significant advantages, since it requires discretization only of the boundary of the vibrating structure. This is particularly attractive for applications aiming to prevent or minimize noise pollution in the early stages of product development. The investigated formulation leads to a space-time linear system, where a specifically chosen set of basis and test functions results in a triangular Galerkin matrix that can be efficiently solved using a block forward substitution. While we demonstrated numerical stability and high accuracy for the calculated sound radiation over long time ranges, involving more than one million time steps for complex automotive gearbox housings, we also observed the computational cost associated with this accuracy. To address this challenge, our current research focuses on reducing the numerical complexity using model order reduction techniques. In particular, we investigate a Laplace Transform Reduced Basis (LT-RB) method, which utilizes solutions of the Laplace-transformed problem, along with proper orthogonal decomposition to extract the most relevant basis functions for spatial reduction. This approach proves to be especially effective when combined with reduced flexible multibody simulations, where structural vibrations, and consequently the Neumann data for the acoustic calculations, exhibit affine-linear behavior. We apply the LT-RB to the acoustic radiation of industrial gearbox housings. The results are validated against experimental measurements in order to assess the accuracy and robustness of the reduction strategy.

**On the Role of Interfaces in Metamaterial Design**

Hermann, Svenja (1); Billon, Kévin (2); Collet, Manuel (2); Madeo, Angela (1)
*1: TU Dortmund, Germany*
*2: École Centrale de Lyon, France*

09:10

In this study, we investigate how different types of interfaces influence the vibration mitigation performance of finite-sized metamaterial structures. The structures are designed in a sandwich configuration in which two homogeneous plates are connected to a metamaterial array. The arrays are based on different unit cells which are cut from the same metamaterial of infinitely large extent. While all the unit cells have identical dispersion relations in the infinitely large metamaterial, strong differences are observed in the vibration response of the finite-sized specimens in experimental measurements and in finite element models.

The observed variations arise from two distinct interface types: material interfaces between the metamaterial arrays and the plates and free interfaces between the metamaterials and surrounding air. These interfaces strongly affect the local displacement fields in the structures and the global vibration transmission. Moreover, the vibroacoustic coupling phenomena that are present in the specimen are found to be dependent on the interfaces.

Based on these findings, optimization strategies that consider not only the metamaterial array but also its adjacent components are proposed. A comparison with benchmark configurations demonstrates that designing the interface can significantly enhance the vibration mitigation performance in finite-sized mechanical metamaterial structures.

**First Order Time Derivative Models in Nonlinear Acoustics**

Lehner, Pascal
*Universität Klagenfurt, Austria*

09:30

Classical models of nonlinear acoustics, such as the Westervelt equation, typically involve secon order time derivatives. In this talk, we present new approaches that lead to models governed solely by first order time derivatives. We further show how these models can be extended to incorporate fractional damping, enabling more realistic descriptions of viscoelastic materials. We conclude with a discussion of well-posedness results for these models in appropriate Sobolev spaces.

## S13: Flow control

Organizer(s): Sesterhenn, Jörn *(Univeristät Bayreuth)*
Giannetti, Flavio *(University of Salerno)*

## S13.01: Flow control

Date: March 19, 2026 14:00–16:00
Room: KII, M17.98

### A roughness-induced drag parameterization and map-based turbulence modeling for channel flows: extended application to barnacle-type roughness

Shampa, Maharun Nesa (1); Medina Méndez, Juan Alí (1); Busse, Angela (2); Klein, Marten (1); Schmidt, Heiko (1)

*1: BTU Cottbus-Senftenberg, Numerische Strömungs- und Gasdynamik, Anwendungszentrum Fluiddynamik, Cottbus, Germany.*
*2: TU Berlin, Numerische Fluiddynamik, Berlin, Germany.*

14:00

Motivated by the apparent success of a recent framework for the map-based modeling of (homogeneous) roughness-induced drag in turbulent channel flows [1], we focus our research effort on drag estimation cases with larger practical relevance. We discuss the quantification of roughness-induced drag in so-called barnacle-type roughness. These types of surfaces are fairly common in ship hulls as a result of marine biofouling. Confident and straightforward application of the framework published in [1] to these types of surfaces is not self-evident. The discussion in [1] introduces two slightly different approaches for the roughness parameterization within the map-based turbulence modeling. The first one is applicable for positively-skewed (Sk > 0) and large effective-slope roughness (ES > 0.35), that is, the peak-dominated, dense roughness surfaces from [2]. The second one is applicable for negatively-skewed (Sk < 0) and small effective-slope roughness (ES < 0.35), which corresponds to the pit-dominated, sparse roughness surfaces from [3]. In contrast to the clearly defined aforementioned represented roughness surfaces, barnacle-type roughness observes a combination of features. We verify whether the suggested framework from [1] is effective in a friction Reynolds number ($Re_\tau$) parametric investigation on a barnacle-type roughness surface, and otherwise quantify the associated prediction errors. The statistically steady turbulent channel flow results obtained using the map-based turbulence model are compared to Direct Numerical Simulation (DNS) data from [4]. The discussion comprises available data on bulk skin friction drag, mean velocity, normal and shear Reynolds stress profiles, as well as a quantification of the roughness function (determined as the downward shift in the mean streamwise velocity profile for a rough wall compared to the smooth-wall at the same $Re_\tau$, as measured by the difference in the centerline velocity values, see [5]). The investigation highlights the nuances and advantages of the use of an economical, dimensionally reduced turbulence modeling framework, which is ideal for parametric investigations typical of engineering design.

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**Investigation of the Friction Coefficient of a Heterogeneous Rough Surface**

Schmitgen, Ute; Schmidt, Carola; Frohnapfel, Bettina 14:20
*Karlsruher Institut für Technologie, Germany*

The investigation and prediction of the friction coefficient (Cf ) of heterogeneous surfaces is the subject of ongoing research. Technical surfaces that exhibit inhomogeneous or heterogeneous roughness lack predictive models for engineering purposes. These surfaces may include river flows, wind over coastlines or urban settlements, biofouling on ship hulls, and corrosion or sediment deposition on pipelines. Since there is an infinite number of forms a heterogeneous rough surface can exhibit, simplifications must be made. However, the database for these simplified surfaces is not extensive enough to make reliable predictions.

This work aims to expand the existing database by presenting data on a simplified surface where smooth and rough patches are aligned to form a checkerboard pattern. This configuration provides an intermediate case between surfaces with spanwise- and streamwise-varying roughness allowing a direct comparison with existing data of these strip arrangements. Using a high-precision blower-type wind tunnel, pressure-drop measurements along the checkered surface are recorded over a wide Reynolds number range. The top and bottom of the channel comprise the checkered surface (width 24 $\delta$); the sides consist of smooth beams (height 2 $\delta$) along which the pressure taps are installed.

In order to investigate the influence of the pressure tap position relative to the checkerboard pattern, measurements are undertaken for two different placements of the pressure taps. These are namely above the edge between two patches, or above the centre of patches. All obtained data show only slight
deviations from each other. This agreement validates the whole measurement approach and enables the comparison with the results from the two striped surfaces, as well as with the two homogeneous cases.

The comparison of the curves show that they all are placed between the curves from the homogeneous surfaces and show similar trends/shape in dependence on the Reynolds number. However, the absolute values differ, even though all curves have the same amount of roughness coverage. Especially, the drag coefficient of the checkerboard surface is not placed between the two striped curves (even though it is the ”combination” of the two of these), but shows a significantly lower drag in the low Reynolds number regime. At high Reynolds numbers, the curve of the streamwise striped and the checkered surface overlap.

The conference contribution will cover the measurement procedure as well as a deeper discussion of the differences and commonalities of the drag results of the different surfaces.

**Impact of Transient Pumping Strategies on Flow Regimes Transitions in Mildly Turbulent Channels**

Polasanapalli, Sai Ravi Gupta (1,2); Klein, Marten (1,2); Schmidt, Heiko (1,2) 14:40
*1: Brandenburgische Technische Universit¨at Cottbus-Senftenber, Germany*
*2: Scientific Computing Lab (SCL), Energie-Innovationszentrum (EIZ), Cottbus, Germany.*

Frictional drag arising from wall shear governs the required pumping power of internal flows. Depending on the application, industrial flows are not always fully turbulent. Slender pipes encountered in industrial-scale heat exchangers or geothermal systems may operate in mildly turbulent or transitional flow regimes, whereas large-scale fluid networks and pipeline systems typically exhibit fully turbulent conditions. A key challenge for operation is that frictional losses in the turbulent regime are significantly higher than in the laminar regime. Several approaches, including surface modifications, polymer additives, and flow relaminarization techniques, have been proposed to reduce turbulent drag. However, these methods often modify fluid properties or wall characteristics, limiting their practical applicability. Recent studies [1, 2] have demonstrated that pulsatile driving of pipe flows using transient pressure gradients and cardiac-cycle-like waveforms can significantly reduce turbulent drag and improve energy efficiency. Unlike conventional methods, this approach achieves drag

reduction by operating pumps in a transient manner without altering fluid or surface properties, but the applicability tends to be currently limited to transitional flow regimes or lower turbulent regimes.

The current work investigates the impact of various transient pressure-gradient profiles on turbulent channel flow that serves as a canonical problem in wall-bounded turbulence. The effects on key parameters such as forcing time period, active pumping duration, and Reynolds number are investigated in the mildly turbulent regime. Three-dimensional numerical simulations have been carried out using the open-source solver Xcompact3d, and the results are compared with a cost-effective standalone map-based stochastic turbulence model [3]. The stochastic model has been developed for fully-developed turbulent flow at high asymptotic Reynolds numbers, but it is demonstrated here that it can extrapolate to low Reynolds numbers, capturing laminarization and transitional behavior.

The talk will discuss the initial findings from both approaches, with a focus on the effect of transient forcing on flow regimes and drag reduction modifications. These findings aim to provide means for efficient numerical modeling and energy-efficient pumping techniques for turbulent internal flows bounded by rigid walls.

References

[1] G. Foggi Rota, A. Monti, M. E. Rosti, M. Quadrio, Scientific Reports 13, 1299 (2023).
[2] D. Scarselli, J. Lopez, A. Varshney, B. Hof, Nature 621, 71 (2023).
[3] S. R. G. Polasanapalli, M. Klein, H. Schmidt, PAMM 24, e202400183 (2024)

**Ferrohydrodynamic Hybrid Nanofluid Flow with Geothermal Viscosity and Slip Effects**

Sharma, Kushal 15:00
*Malaviya National Institute of Technology Jaipur, India*

Efficient heat transfer is essential for the reliability and performance of modern engineering and electronic systems. To enhance the thermal efficiency of conventional fluids, this study investigates the ferrohydrodynamic flow of a hybrid nanofluid between co-rotating coaxial disks, considering slip, Soret, and Dufour effects. Kerosene oil is selected as the base fluid, while nickel–zinc ferrite and manganese–zinc ferrite nanoparticles are suspended to enhance thermal transport. Using similarity transformations, the governing equations are reduced to a system of nonlinear ordinary differential equations, which are then solved numerically using Maple software to examine the influence of key parameters on velocity and temperature profiles. The results show that the hybrid nanofluid provides significantly higher heat transfer performance than the single-particle nanofluid. The findings are directly applicable to biomedical systems, nano-drug delivery, thermal devices, and manufacturing processes.

**Control of Bénard–Marangoni Instability by Periodic Thermal Forcing in Superposed Fluid–Porous Layers**

RASTOGI, TANYA; SUTHAR, OM 15:20
*Malaviya National Institute of Technology Jaipur, India*

This study investigates convective instability in a superposed system consisting of a Darcy porous layer filled with glass beads beneath a water layer with a stress-free free surface incorporating surface tension effects. The porous layer is subjected to time-periodic heating at its lower boundary, while at the upper free surface a mixed thermal boundary condition is imposed. Coupling between the fluid and porous layers is modeled using the Beavers–Joseph–Saffman–Jones interface condition. By employing a Fourier expansion in the horizontal direction and the Chebyshev tau method in the vertical direction, the governing equations are reduced to a generalized eigenvalue problem whose eigenvalues determine the stability of the time-periodic system. Validation is achieved by considering limiting values of the fluid-to-porous depth ratio, which recover the classical Bénard–Marangoni configuration. The results demonstrate that periodic heating can effectively control the onset of Marangoni and coupled Rayleigh–Marangoni instabilities, particularly for thin fluid layers overlying porous substrates. Appropriate choice of modulation parameters allows the instability region to be shifted between the fluid

layer, the porous layer, or the entire system, thereby enabling stability control without altering the physical configuration.

## S13.02: Flow control

Date: March 20, 2026 08:30–10:30
Room: KII, M17.98

### A Hybrid-Airfoil Strategy for Improving Off-Design Performance and Stability of a Small-Scale Wind Turbine

Laouar, Roudouane (1); Bekkai, Riyadh (1); Wünsch, Olaf (2) 08:30
*1: Echahid Cheikh Larbi Tebessi university, Algeria*
*2: Universität Kassel, Institut für Mechanik, Fachgebiet Strömungsmechanik*

This study investigates a hybrid-airfoil strategy to improve the aerodynamic stability and off-design robustness of a small-scale horizontal axis wind turbine, the 1.5 m Anderson rotor, under low-Reynolds-number conditions. A broad set of hybrid configurations were tested in QBlade by combining SG6043 and SG6040 profiles along the wingspan. The best configuration, featuring a balanced root-tip transition, demonstrated superior performance not only over the clean reference airfoil but also over the mixed, non-hybrid baseline blade, ensuring a fair and physically meaningful comparison. High-fidelity CFD simulations using the SST k–$\omega$model were then employed to isolate and visualize with high accuracy the aerodynamic benefits of hybridization: the optimized hybrid rotor exhibits more coherent streamlines, delayed and reduced separation near the root and tip, smoother and more uniformly distributed pressure fields across the entire TSR range. These flow-physics improvements translate into measurable performance gains, including earlier start-up, stronger off-design efficiency, reduced aerodynamic loading, and enhanced operational resilience. By combining the complementary strengths of the two airfoils into intelligent, functionally graded blade sections, the hybrid rotor achieves higher energy extraction and improved structural reliability. The demonstrated superiority compared to non-hybrid rotors, whether pure or mixed, positions hybridization as a promising and physically sound path for the design of next-generation rotors and an essential direction for advanced aerodynamic research.

### Deterministic Data Assimilation for Compressible Jets Using Schlieren Imaging and DNS

Farhikhteh, M. Erfan; Sesterhenn, Jörn 08:50
*University of Bayreuth, Germany*

Data assimilation provides an effective way to reconstruct incomplete flow fields by combining experimental measurements with numerical simulations. In this work, deterministic data assimilation methods are applied to compressible jet flows using two-dimensional Schlieren imaging data and three-dimensional direct numerical simulation (DNS) results. The objective is to recover physically meaningful density fields from limited projection-type measurements and to investigate how constraints and regularization improve the stability and quality of the reconstruction.

The study begins with a standard least-squares formulation, where projected density data derived from Schlieren images are assimilated to reconstruct a two-dimensional density field. The inverse problem is solved iteratively using a conjugate-direction method. Although the residual decreases steadily to very small values, the unconstrained solution is sensitive to noise and fails to reproduce realistic flow structures.

To address these limitations, additional constraints are introduced. A global mean-value constraint is first applied to correct bias in the reconstructed density field, improving the overall amplitude but providing limited enhancement of spatial details. A Laplacian constraint is then added to control curvature and suppress non-physical oscillations. This regularization leads to smoother reconstructions that better capture large-scale jet features and shear-layer structures observed in the Schlieren data.

The methodology is further extended to three-dimensional DNS jet data using a Karush–Kuhn–Tucker (KKT) formulation. This approach enforces the data misfit and physical constraints simultaneously

within a single system. Compared to unconstrained and penalty-based methods, the KKT formulation yields improved agreement with projected measurements.

Overall, the results demonstrate that constraint-based regularization is essential for Schlieren-based data assimilation and that KKT formulations provide a notable framework for reconstructing compressible flows from limited measurements.

**Hybrid Screening–MOGA Refinement for High-Fidelity Wind Turbine Blade Optimization**

Bekkai, Riyadh (1); Laouar, Roudouane (1); Wünsch, Olaf (2)
*1: Echahid Cheikh Larbi Tebessi university, Algeria*
*2: Universität Kassel, Institut für Mechanik, Fachgebiet Strömungsmechanik*

09:10

This work presents a hybrid optimization framework combining global Screening with a locally refined MOGA strategy to improve wind turbine blades performance under high-fidelity CFD analysis. Starting from a baseline rotor and a design of experiments of 50 CFD simulations, a global Kriging surrogate model is built to describe the overall aerodynamic response.

The Screening stage is used to isolate the most influential and high-potential regions of the design space, which are then exploited through a locally constrained MOGA refinement. This targeted hybridization enables an efficient and focused exploration of promising regions without modifying the initial experimental design (DOE) or the surrogate model.

The proposed hybrid strategy outperforms Screening and MOGA approaches taken individually. CFD-based analyses reveal that the optimized blade exhibits reduced flow separation near the trailing edge and better flow adhesion on the rotor surface, resulting in improved aerodynamic behavior. Performance improvements are confirmed across the entire range of tip-speed ratios (TSR), where the hybrid design systematically outperforms the baseline rotor.

Overall, the hybrid framework demonstrates faster convergence, improved robustness, and superior aerodynamic performance, thanks to physically meaningful flow mechanisms rather than purely numerical optimization. The methodology provides an efficient and reliable pathway for CFD-driven wind turbine blade optimization, offering a valuable contribution to advanced rotor design under realistic flow conditions.

**Reduced Order Modelling and Optimal Flow Control Strategies for Hemodynamics**

Rozza, Gianluigi
*SISSA, Italy*

09:30

Accurate numerical simulations of the cardiovascular system play a crucial role in the diagnosis and surgical planning of vascular diseases. However, the reliability of these simulations is often compromised by parameter uncertainty and the large computational cost associated with high-fidelity 3D models. Our works study integrated frameworks for optimal flow control problems (OCPs) governed by the incompressible Navier-Stokes equations, with a focus on biomedical applications such as coronary artery bypass grafts and drug delivery systems.
The proposed approach leverages adjoint-based Lagrangian methodologies to derive optimality conditions. To overcome the prohibitive computational demands of real-time and many-query scenarios, we investigate different Reduced Order Methods (ROMs). These include projection-based techniques such as Proper Orthogonal Decomposition (POD) combined with Galerkin projection, as well as non-intrusive data-driven approaches. We address the challenge of defining realistic boundary conditions, where outflow stresses or inflow rates are calibrated to minimize the mismatch between numerical results and target clinical data. Computational results on both idealized and patient-specific geometries demonstrate that the implemented ROMs effectively capture the flow dynamics while achieving significant computational speed-ups compared to full order simulations. The flexibility of the proposed frameworks is further showcased through applications in time-dependent flow regimes and parametric studies involving varying Reynolds numbers, providing valuable insights into clinical indicators such as the wall shear stress. The combination of OCPs and model reduction offers a robust path toward personalized, real-time computational tools for clinical decision support.

## S14: Applied analysis

Organizer(s): Engl, Dominik *(KU Eichstätt-Ingolstadt)*
Düll, Wolf-Patrick *(Universität Stuttgart)*

## S14.01: Applied analysis

Date: March 17, 2026 08:30–10:30
Room: KII, M17.23

### Homogenization of a rate-independent delamination model with random geometry

Thomas, Marita (1); Heida, Martin (2); Schütz, Leon (3)
*1: Freie Universität Berlin, Germany*
*2: Weierstrass Institute for Applied Analysis and Stochastics*
*3: –*

08:30

We study an elastic compound that is exposed to rate-independent delamination processes along prescribed interfaces. The interfaces are described by polyhedra of random geometry. By means of stochastic two-scale homogenization we deduce a macroscopic phase-field model for rate-independent volume-damage of Ambrosio-Tortorelli-type.

### Rate dependent dislocation dynamics and gradient flows of currents

Češík, Antonín (1); Hudson, Thomas (1); Kampschulte, Malte (2); Rindler, Filip (1)
*1: University of Warwick*
*2: Charles University Prague, Faculty of Mathematics and Physics*

08:50

Dislocation dynamics describes the movement of defects in the crystaline structure of a material. Like many problems related to geometry, it can be mathematically modelled as movement of manifolds. In the simplest case, this movement has the structure of an abstract gradient flow, involving an $L^p$-type distance. However, due to the low regularity of objects involved, it has been long understood that, for any naive description, in the rate-dependent case p>1, such a distance is always mathematically degenerate. So far this resulted either in nonsensical solutions or in distances that lacks the properties required to prove existence.
The abstract part of this talk will recapitulate the problems of a naive approach and then introduce a new natural notion of distance and solution, which mixes ideas from currents and Young-measures to achieve otherwise unavailable lower semi-continuity. This in turn allows us to show existence of solutions using well known methods. The applied part will show how these results can be related to certain phenomena of dislocation dynamics in plasticity and also give further applications in problems related to mean curvature flow.

### Perturbed Minimizing Movements of Time-Dependent Functionals on Metric Spaces

Götzmann, Gianna (1); Pietschmann, Jan-Frederik (1); Tribuzio, Antonio (2)
*1: University of Augsburg*
*2: University of Bonn*

09:10

Minimizing movement schemes are a fundamental tool to approximate evolution equations that have a gradient-flow structure with respect to an energy or entropy functional $\mathcal{F}$ such as the Fokker–Planck equation describing drift–diffusion processes. With the aim of treating homogenization problems involving, for instance, a geometry that evolves in time, we consider a perturbation of the functional in the sense of a $\Gamma$-converging sequence $\mathcal{F}_\varepsilon$, as well as a time dependence. That is, our scheme includes a time discretization $\mathcal{F}_{\varepsilon,\tau,n}$, $n = 1, \dots, N$, of $\mathcal{F}_\varepsilon$ where $N$ is the number of time steps and $\tau$ is the step size. We study the case where $\varepsilon$ and $\tau$ tend to $0$ simultaneously and establish sufficient conditions to obtain minimizing movements in the limit.

**The dynamic Schrödinger problem on metric graphs**

Krautz, Juliane (1); Pietschmann, Jan-F. (1,2)
*1: University of Augsburg, Germany*
*2: Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg*

09:30

In this talk, we discuss the dynamic formulation of the Schrödinger problem on metric graphs. Using the
Direct Method of Calculus of Variations we show existence of minimizers and investigate the connection to dynamic Optimal Transport. A particular focus lies on the study of $\Gamma$-convergence between both problems for vanishing diffusive effects.

**Hölder Regularity of Solutions to the Beckmann Problem with Quadratic Cost**

Gottschalk, Hanno; Riedlinger, Tobias
*Technische Universität Berlin, Germany*

09:50

Beckmann's problem in optimal transport minimizes the total squared flux in a continuous transport problem from a source to a target distribution. In this article, the regularity theory for solutions to Beckmann's problem in optimal transport is developed utilizing an unconstrained Lagrangian formulation and solving the variational first order optimality conditions. It turns our that the Lagrangian multiplier that enforces Beckmann's divergence constraint fulfills a Poisson equation and the flux vector field is obtained as the potential's gradient. Utilizing Schauder estimates from elliptic regularity theory, the exact Hölder regularity of the potential, the flux and the flow generating is derived on the basis of Hölder regularity of source and target densities on a bounded, regular domain. We show that this approach can be generalized to suitably regular probability paths like Fisher-Rao gradient flows by means of the theory of interpolation spaces. A further generalization involves a parametric dependency with a suitable regularity arising in conditional generative learning problems.

## S14.02: Applied analysis

Date: March 17, 2026 16:30–18:30
Room: KII, M17.23

**Homogenization of nonlocal exchange energies in micromagnetics**

Giorgio, Rossella (1); Happ, Leon (2); Schönberger, Hidde (3)
*1: Technische Universität Wien, Austria*
*2: Universidad Autónoma de Madrid, Spain*
*3: Université catholique de Louvain, Belgium*

16:30

We study the homogenization of nonlocal micromagnetic functionals incorporating both symmetric and antisymmetric exchange contributions under the physical constraint that the magnetization field takes values in the unit sphere. Assuming that the nonlocal interaction range and the scale of heterogeneities vanish simultaneously, we capture the asymptotic behavior of the nonlocal energies by identifying their $\Gamma$-limit, leading to an effective local functional expressed through a tangentially constrained nonlocal cell problem. Our proof builds upon a tailored notion of two-scale convergence, which takes into account oscillations only in specific directions. It enables us to describe the two-scale limit of suitable nonlocal difference quotients, yielding a nonlocal analog of the classical limit decomposition result for gradient fields. To deal with the manifold constraint of the magnetization, we additionally prove that the microscopic oscillations in the two-scale limit are constrained to lie in the tangent space of the sphere.

**Variational derivation of membrane models from three-dimensional anisotropic nonlocal hyperelasticity**

Doležalová, Anna (1); Engl, Dominik (2); Molchanova, Anastasia (3); Schönberger, Hidde (4) 16:50

*1: UTIA, Czech Academy of Sciences, Czech Republic*
*2: KU Eichstätt-Ingolstadt, Germany*
*3: University of Vienna, Austria*
*4: UCLouvain, Belgium*

Nonlocal derivatives with finite horizon have so far been defined through interaction kernels supported on balls of positive radius. In this work, we propose an anisotropic generalization in which the interaction region is an axis-aligned ellipsoid whose principal radii may even vanish independently of each other. This provides a unified framework that interpolates between fully nonlocal, partially nonlocal, and purely local models. Motivated by the analysis of thin structures, we incorporate this anisotropic nonlocal derivative into nonlocal hyperelastic energies and carry out a variational dimension reduction to a membrane model. The limit functional retains the structural form of the classical membrane energy, and the classical local model is recovered precisely when all interaction radii vanish. This is joint work with Anna Doležalová, Anastasia Molchanova and Hidde Schönberger.

**A general compactness result for localization of nonlocal gradients**

Kreisbeck, Carolin (1); Mora-Corral, Carlos (2); Seifert, Felix (1) 17:10

*1: KU Eichstätt-Ingolstadt, Germany*
*2: Universidad Autónoma de Madrid*

Localization results provide a rigorous way to relate nonlocal models to their local counterparts. In the context of variational models, $\Gamma$-convergence together with the necessary compactness results offers the natural framework for analyzing such limit processes. In this talk, we discuss this approach for problems in which nonlocality arises through nonlocal gradients, as in models of nonlocal hyperelasticity. Whereas previous works often focused on kernels resulting from a specific construction, such as rescaling, or on special classes, like fractional kernels, we instead consider arbitrary sequences of radial kernels that satisfy suitable localization, monotonicity, and regularity conditions. This yields a more general approach that both encompasses various earlier results and extends them further, in particular by allowing for kernels with unbounded support and even non integrable kernels. The main technical difficulty lies in the proof of compactness, which relies on establishing a nonlocal Poincaré inequality with uniform constants, as well as a uniform continuous embedding into a nonlocal Sobolev space given by a fractional reference kernel. To illustrate the scope of our results, we will show how different relevant examples fit into this setting. This is joint work with Carolin Kreisbeck (KU Eichstätt-Ingolstadt) and Carlos Mora-Corral (Universidad Autónoma de Madrid).

**Peridynamic Modeling of Process-Dependent Material Strength in Additive Manufacturing**

Willberg, Christian (1); Hesse, Jan-Timo (2) 17:30

*1: Magdeburg-Stendal University of Applied Sciences, Germany*
*2: German Aerospace Center Braunschweig, Germany*

Additive manufacturing (AM) enables the fabrication of complex geometries with unprecedented design freedom. However, the mechanical properties and failure behavior of AM components are highly sensitive to process parameters such as temperature history, printing speed, and path planning.

This work presents an efficient peridynamic simulation framework for predicting how manufacturing processes influence the mechanical behavior of AM parts. Using our open-source platform PeriLab, we implement a multiphysics model that simulates the complete process chain: layer-by-layer deposition, thermal history, and polymer curing kinetics. The manufacturing simulation captures how process parameters affect the resulting material properties and residual stress states.

Subsequently, we perform virtual tensile tests on the simulated specimens to analyze their failure behavior. An energy-based damage model enables the prediction of crack initiation and propagation without predefined crack paths. Our results demonstrate that variations in manufacturing conditions

lead to changes in fracture toughness, crack growth rates, and failure modes, revealing clear process-property-failure relationships.

The presented peridynamic formulation naturally couples thermal and mechanical physics while capturing the influence of manufacturing history on subsequent mechanical performance. These findings provide quantitative insights for optimizing AM processes to achieve targeted mechanical properties and structural reliability.

**Asymptotic analysis of thin plates with disconnected rigid inclusions**

Chakrabortty, Amartya (1); Griso, Georges (2); Orlik, Julia (1)

*1: Fraunhofer ITWM, Germany*

*2: Laboratoire Jacques-Louis Lions (LJLL), Sorbonne Université, CNRS, Université de Paris, F-75005 Paris, France.*

17:50

We present the simultaneous homogenization and dimension-reduction limit for thin composite plates with periodically distributed rigid inclusions, with emphasis on the nonlinear elastic regime. The reference configuration is a connected, periodically perforated elastic matrix whose holes are filled with rigid substructures. The thickness parameter $\delta$is asymptotically smaller than the periodicity $\varepsilon$, namely $0 < 3\delta < \varepsilon < 1$ and $\delta/\varepsilon \to 0$ as $(\varepsilon, \delta) \to (0, 0)$, so that high-contrast effects and plate reduction occur in a coupled multiscale limit. In nonlinear elasticity, rigidity in the inclusions is modeled by the constraint $\nabla v \in SO(3)$ in the rigid phase, while the soft matrix stores elastic energy. We establish a decomposition of admissible deformations adapted to the composite geometry: each deformation is split into an elementary part satisfying the rigid constraint and a residual term, using geometric rigidity and Q1 interpolation. This yields uniform estimates under an energy scaling above the classical von Kármán order but below the large-deformation regime. To capture the coupled limits $\varepsilon \to 0$ and $\delta \to 0$, we employ rescaled unfolding operators to characterize the limiting behavior of nonlinear strain tensors and derive the effective model via $\Gamma$-convergence. The limiting theory is a homogenized constrained von Kármán plate model: the limit displacement U = (U1, U2, U3) satisfies first-order infinitesimal isometry constraints, and the limit energy is finite only on the constrained class $e_{\alpha\beta}(U) + \frac{1}{2}(\partial_\alpha U_3)(\partial_\beta U_3) = 0$, and $\partial_{12} U_3 = 0$ in $\omega$, reflecting the mechanical influence of the rigid inclusions on bending. The homogenized quadratic form is characterized through cell problems and correctors, and we prove the existence of minimizers together with a recovery sequence, completing the $\Gamma$-convergence analysis. For comparison, the linearized counterpart yields a Kirchhoff–Love limit displacement.

**Periodicity in the Double Gradient Model for Phase Transitions**

Deutsch, Jakob

*TU Wien, Austria*

18:10

We investigate the limsup inequality in the double gradient model for phase transitions governed by a Modica-Mortola functional with a double-well potential in two dimensions. Assuming a bound on the optimal profile constant — namely, the cell problem on the unit cube — in terms of the geodesic distance between the two wells, we characterize the limiting interfacial energy via periodic recovery sequences.

## S14.03: Applied analysis

Date: March 18, 2026 14:00–16:00

Room: KII, M17.23

**On the validity of amplitude equations for systems with noise**

Schneider, Guido; Logioti, Anna

*Universität Stuttgart, Germany*

14:00

Amplitude equations, such as the Ginzburg-Landau equation or the KdV equation, can be derived using a multiscale approach to describe more complicated systems.
Numerous approximation results have been proven in the last decades.

In the lecture, the question will be addressed which of these deterministic results remain valid in the case of additional noise.

**On the Ginzburg-Landau approximation for quasilinear pattern forming reaction-diffusion-advection systems**

Belin, Théo
*University of Stuttgart, Germany*

14:20

In this talk, I will show that the Ginzburg-Landau equation correctly predicts the dynamics of quasilinear pattern-forming reaction-diffusion-advection systems, close to the first instability where a Turing bifurcation occurs. I will present a simple functional analytic framework, where an optimal regularity result on the linearized operator gives the wanted bound for the error between the solution of the system and the solution of the Ginzburg-Landau equation on a long timescale. The approximation result is applied to the generalized Klausmeier-Gray-Scott model describing the water-vegetation interaction in semi-arid regions.

**Justification of the Nonlinear Schrödinger and the Davey-Stewartson Approximation for the Three-Dimensional Water Wave Problem With and Without Surface Tension**

Düll, Wolf-Patrick; Schewe, Franz
*Universität Stuttgart, Germany*

14:40

We consider the three-dimensional water wave equations in an infinite domain with finite or infinite depth of water and with or without surface tension. This system has wave-packet like solutions whose envelopes can formally be approximated by solutions to the Nonlinear Schrödinger equation in the case of infinite depth, or solutions to the Davey-Stewartson system in case of finite depth. While it was already shown that analogous approximations can be rigorously justified for the two-dimensional water wave problem, only approximation results for infinite depth and no surface tension exist in three dimensions.
In this talk, we discuss the rigorous justification for the three-dimensional water wave problem in isothermal coordinates with and without surface tension by error estimates over a physically relevant time span. The estimates are uniform as the surface tension tends to zero. Additional resonances that arise in three dimensions are handled in order to obtain estimates on the required time scale. For the error estimates, we use a new systematic approach taking advantage of the Hamiltonian structure of the original system.

**Time-asymptotic Self-similarity of the Damped Euler Equations in Parabolic Scaling Variables**

Eiter, Thomas (1,2); Schindler, Stefanie (1)
*1: Weierstrass Institute, Germany*
*2: Freie Universität Berlin*

15:00

In this talk, we investigate the long-time behavior of solutions to the compressible Euler equations with frictional damping on the real line, where we prescribe nonzero values for the density at spatial infinity. To this end, we transform the system into parabolic scaling variables and derive a relative entropy inequality, which allows to conclude the convergence of the density towards a self-similar solution to the porous medium equation while the associated limit momentum is governed by Darcy's law.

**A relative energy inequality for an anisotropic Navier–Stokes–Nernst–Planck–Poisson system weak-strong uniqueness and a posteriori error estimates**

Lasarzik, Robert; Plato, Luisa
*Weierstrass Institute, Germany*

15:20

In this talk, I build upon the framework of suitable weak solutions to the anisotropic Navier–Stokes–Nernst–Planck–Poisson (NSNPP) system and establish a relative energy inequality for

these solutions. This inequality serves as the basis for proving the weak-strong uniqueness property. Additionally, it can be exploited as a tool to obtain a posteriori error estimates. We are interested in the high-viscosity-low-Reynolds number limit of the NSNPP, which leads to the anisotropic Stokes–Nernst–Planck–Poisson (SNPP) system. Utilizing the relative energy framework, we derive an error estimate for the distance between solutions to the NSNPP and SNPP model in natural energy and dissipation norms.

## S14.04: Applied analysis

Date: March 18, 2026 16:30–18:30
Room: KII, M17.23

### Inner-Layer Asymptotics in Partially Perforated Domains: Coupling Across Oscillating Interface

Melnyk, Taras 16:30
*University of Stuttgart, Germany*

This talk addresses the asymptotic analysis of boundary-value problems in domains that combine perforated and imperforate regions. We consider a porous medium with symmetric, periodic microstructure of small period $\varepsilon$, where Neumann conditions are imposed on the perforation boundaries. A central challenge lies in deriving correct coupling conditions across the common interface, which we resolve using inner-layer asymptotics. For the case of a flat interface, we construct and rigorously justify a complete asymptotic expansion of the solution in the Sobolev space $H^1(\Omega_\varepsilon)$. When the interface oscillates with period $\varepsilon$ and amplitude of order $\mathcal{O}(\varepsilon)$, we develop an approximation that captures the influence of the oscillations in the second-order term of the expansion and establish corresponding asymptotic estimates in $H^1$-Sobolev spaces. The results highlight how oscillatory geometry modifies coupling conditions and enriches the homogenized description of partially perforated domains.

### Homogenization of viscoelastic non-simple materials at large strains

Gahn, Markus 16:50
*University of Augsburg, Germany*

In this talk, we perform the homogenization for nonlinear viscoelastic non-simple perforated materials at large strain in the quasistatic setting. Starting from a microscopic model on a periodically perforated reference domain depending on a scaling parameter $\varepsilon$ giving the ratio between the size of the whole domain and the small periodic perforations, for $\varepsilon \to 0$ we rigorously derive a macroscopic model including homogenized coefficients. The mechanical energy in the micro-model depends on both, the gradient and the second gradient of the deformation, and also respects positivity of the determinant of the deformation gradient. Further, we assume dynamic frame indifference for the viscous stresses. For the homogenization we use the two-scale convergence and the unfolding method. The most crucial step is to establish $\varepsilon$-uniform a priori estimates for the microscopic solutions, in particular for the rate of the deformation gradient. For this we construct new extension operators for second order Sobolev spaces and prove a Korn inequality for non-constant coefficients on the perforated domain. Another crucial aspect is to guarantee an $\varepsilon$-independent positive lower bound for the determinant of the deformation gradient.

### Effective interface laws of Navier-slip-type involving the elastic displacement for Stokes flow through a thin elastic porous layer

Gahn, Markus (1); Neuss-Radu, Maria (2) 17:10
*1: University of Augsburg, Germany*
*2: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

This contribution presents a rigorous derivation of an effective model for fluid flow through a thin elastic porous membrane separating two fluid bulk domains. The membrane is composed of a solid phase and fluid-filled pores, with thickness and periodicity of order $\varepsilon$, small compared to the size of

the bulk regions. The microscopic model is governed by a coupled fluid-structure interaction system, with two distinct scalings of the elastic stress tensor.

Using two-scale convergence techniques adapted to thin domains and oscillatory microstructures, the membrane is reduced to an effective interface across which transmission conditions are derived. The macroscopic model couples the fluid bulk domains via effective interface laws of Navier-slip-type including the dynamic displacement. This coupling depends critically on the scaling in the elastic stress tensor, leading to either a membrane equation or a Kirchhoff-Love plate equation for the effective displacement. For the derivation of these effective models, cell problem techniques are employed systematically to construct admissible test-functions and to rigorously extract the effective coefficients. The resulting interface conditions naturally admit mass exchange between the adjacent fluid regions.

**Homogenization of a Stokes-transport system in an anisotropic porous medium with thin, evolving tubes**

Gahn, Markus (1); Hacker, Kilian (2); Neuss-Radu, Maria (2) 17:30

*1: Universität Augsburg, Germany*
*2: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

In this contribution, we study the asymptotic behavior of a Stokes flow in an array of thin, evolving tubes, coupled with advective-diffusive transport within the tubes and in the surrounding medium. The domain evolution is induced by the transport process via chemical reactions at the microscopic lateral boundaries of the tubes, leading to a fully coupled problem. Our approach aims to model the thermal control of blood flow in human skin, including temperature-dependent production of biochemical substances and the subsequent dilation and constriction of blood vessels.
After a transformation of the microscopic problem onto a periodic microscopic reference domain, we rigorously derive a fully coupled effective model, by means of the methods of homogenization. It consists of an anisotropic Darcy model coupled to an effective reaction-diffusion-advection system of partial and ordinary differential equations. The effective coefficients (permeability, diffusivity) of the macroscopic model are computed from solutions to standard cell problems involving the time and space dependent macroscopic deformation gradient. The anisotropies induced by the special features of the geometry (array of thin tubes) are exhibited in the effective model.

**Effective transmission through an interface with evolving microstructure**

Fix, Lucas M. (1); Götzmann, Gianna (1); Peter, Malte A. (1,2); Pietschmann, Jan-F. (1,2) 17:50

*1: University of Augsburg, Germany*
*2: Centre for Advanced Analytics and Predictive Sciences (CAAPS), Germany*

We study the asymptotic behaviour of a system of nonlinear reaction–diffusion–advection equations in a domain consisting of two bulk regions connected via microscopic channels distributed within a thin membrane. Both the width of the channels and the thickness of the membrane are of order $\varepsilon \ll 1$, and the geometry evolves in time in an a priori known way. We consider nonlinear flux boundary conditions at the lateral boundaries of the channels and critical scaling of the diffusion inside the layer. Extending the method of homogenisation in domains with evolving microstructure to thin layers, we employ two-scale convergence and unfolding techniques in thin layers to derive an effective model in the limit $\varepsilon \to 0$, in which the membrane is reduced to a lower-dimensional interface. We obtain jump conditions for the solution and the total fluxes, which involve the solutions of local, space–time-dependent cell problems in the reference channel.

**A thermodynamically consistent approximation of the Navier–Stokes–Cahn–Hilliard system for incompressible two-phase flows**

Konan, Hasel Cicek; Rohde, Christian
*IANS, Germany*

18:10

Diffuse-interface models describe topological changes between immiscible or partially miscible fluids and have gained increasing attention for the simulation of two-phase flows. In this work, we consider a diffuse-interface model for two incompressible and immiscible fluids at a constant temperature. To investigate the interface dynamics of such flows, we focus on the incompressible Navier–Stokes–Cahn–Hilliard (NSCH) system, which is thermodynamically consistent. Despite its modeling advantages, the NSCH system is computationally expensive due to the presence of nonlocal nonlinear terms, the fourth-order Cahn–Hilliard equation, and the pressure Poisson problem.

To overcome these challenges, we introduce a first-order hyperbolic approximation of the inviscid part of the NSCH system. This approximation preserves thermodynamic consistency while enabling the use of standard numerical methods for hyperbolic balance laws and reducing computational cost by avoiding fourth-order derivatives and the pressure Poisson equation. A characteristic analysis of the hyperbolic approximation in one spatial dimension yields asymptotic expressions for four real and distinct eigenvalues, which are derived up to a prescribed asymptotic order.

To validate the hyperbolic relaxation, numerical experiments are performed in one spatial dimension. We employ a classical second-order finite-volume MUSCL–Hancock scheme with a Rusanov numerical flux. The numerical results accurately capture the wave structure of the hyperbolic part of the approximate system. In addition, we consider three benchmark test cases: a stationary droplet, spinodal decomposition, and Ostwald ripening. The results demonstrate the convergence of the approximate solutions toward the original NSCH solution as the relaxation parameters tend to zero. We further show that the proposed numerical schemes are energy dissipative for all test cases. Finally, a comparison of computational costs for the stationary droplet benchmark confirms the efficiency of the hyperbolic approximation.

## S14.05: Applied analysis

Date: March 19, 2026 08:30–10:30
Room: KII, M17.23

**On solutions to a model for slightly compressible, visco-elasto-plastic deformation**

Eiter, Thomas (1,2)
*1: Freie Universität Berlin, Germany*
*2: Weierstrass Institute for Applied Analysis and Stochastics, Berlin, Germany*

08:30

We study a model for the deformation of a visco-elasto-plastic material that is nearly incompressible. It is given in Eulerian description and combines a Kelvin-Voigt rheology in the spherical part with a Jeffreys-type rheology in the deviatoric part. Despite a constant density, an adapted momentum equation allows for non-isochoric deformation and the propagation of pressure waves. This is coupled with an evolution equation for the small elastic strain, in which plasticity is modeled through a non-smooth dissipation potential. Since the well-posedness in a weak setting cannot be expected, we study two possible modifications: the regularization by an additional diffusive term, and the relaxed concept of energy-variational solutions. In both cases, solutions are constructed by the same time-discrete scheme, consisting of solving a saddle-point problem in each time step.

**Morphoelastic Growth at Large Strains**

Blawid, Julian; Dolzmann, Georg
*University of Regensburg, Germany*

08:50

We discuss a model for morphoelastic growth of second gradient viscoelastic materials. Morphoelastic growth refers to the growth of tissue under the influence of elastic stress. Our model features a multiplicative decomposition of the deformation gradient into a part related to growth and an elastic

contribution. While the volumetric change due to growth of the tissue is determined by an ordinary differential equation on a Banach space, the total deformation solves a quasistatic momentum balance equation. The growth process is driven by the absorption of nutrients, the concentration of nutrients is modeled by the solution of a parabolic reaction-diffusion equation.

**Qualitative properties of solutions of transmission problems for arch beams with thermal damping.**

Fastovska, Tamara (1,3); Langemann, Dirk (2)
*1: Humboldt-Universität zu Berlin*
*2: Technische Universität Braunschweig*
*3: V.N. Karazin Kharkiv National University*

09:10

We investigate dynamical systems generated by nonlinear partial differential equations describing the dynamics of two initially curved beams in rigid contact, with thermal damping acting on one of the beams [1]. We establish the existence of compact global attractors for these systems and analyze their structure under certain assumptions on the problem parameters. Furthermore, we study singular limits in two scenarios: when the beam curvature tends to zero, and when the curvature tends to zero simultaneously with the shear moduli approaching infinity.

**References**

[1] T. Fastovska, D. Langemann, On the asymptotic properties of solutions to a nonlinear transmission problem for a Bresse beam with thermal damping, Evolution Equations and Control Theory (2025), 1-47, 10.3934/eect.2026002.

**The fuzzy Landau equation: global well-posedness and Fisher information**

Gualdani, Maria Pia (1); Guillen, Nestor (2); Pavlović, Nataša (1); Tasković, Maja (3); Zamponi, Nicola (4)
*1: The University of Texas at Austin, Austin, TX 78712, USA*
*2: Texas State University, San Marcos, TX 78666, USA*
*3: Emory University, Atlanta, GA 30322, USA*
*4: Universität Augsburg, 86159 Augsburg, Germany*

09:30

We study a fuzzy variant of the inhomogeneous Landau equation and establish global-in-time existence and uniqueness of smooth solutions for moderately soft potentials. The spatial delocalization introduced in the collision operator not only enhances regularity and prevents singularity formation, but also reveals additional structural properties of the model. In particular, we show that several forms of the Fisher information decay monotonically or remain uniformly bounded in time.

**Drift-diffusion models with Schottky contacts at metal-semiconductor interfaces**

Glitzky, Annegret; Liero, Matthias
*Weierstrass Institute, Germany*

09:50

This talk deals with the analysis of drift-diffusion models for semiconductor heterostructures with Schottky contacts at metal-semiconductor interfaces. Here, we assume that no additional Dirichlet contacts are present. Such situations occur, for example, in memristive devices, which are two-terminal electrical devices whose resistance depends on the history of charge flow in the device. Integrated circuits of such devices should combine data processing and storage and be suitable for neural networks.

Our analytical investigations allow for Boltzmann as well as Fermi–Dirac statistics for the charge carrier densities. We verify the existence and boundedness of weak solutions of the instationary van Roosbroeck system in this context. We work with the related free energy functional, consider appropriate regularizations, and

apply time discretization to first solve the regularized problem. Next, Moser iteration techniques ensure the desired upper and lower estimates of the charge carrier densities. Moreover, under additional assumptions, the uniqueness and the higher regularity of the solution are demonstrated. Here, results of higher regularity for scalar quasilinear parabolic partial differential equations are used.

**Can tachyon solutions of sine-Gordon equation contribute to dark energy**
Günther, Helmut
*Fachhochschule Bielefeld, Germany*
10:10

As "Faster Than Light P?articles" G. Feinberg introduced Tachyonsd in 1967 .

In1966 and 2000 we have expülaine how these Tachyons are embedded in ther formalism of Speciual Relativity and then exermined the question of their real existence. The charactertiostic quantity for Tachyons is their momentum parametert instead of the restmass of particles. And we pointed out trhe differtent between the term correlatioons and interacriomn. We find tachyons as solutions of an nonlinear partial differential equation, the so-called sine-Gordon equation over a lattice structure, what was first suggested by g. Eilenberger 1981.As outlined in detail in "Tachyons and Relativity", ISBN 976364409083, we discussed tachyons moving nesr the velocity of light, so that their increasing energy may explain dark energy.

## S14.06: Applied analysis
Date: March 19, 2026 14:00–16:00
Room: KII, M17.23

**Weak-Strong Uniqueness and Relaxation Limit for a Parabolic Relaxation of the Navier-Stokes-Korteweg System**
Wendt, Florian
*University of Stuttgart, Germany*
14:00

In this talk, we consider a parabolic relaxation formulation for the compressible Navier-Stokes-Korteweg system. This relaxation model depends on two positive relaxation parameters $\alpha$, $\beta > 0$ and approximates formally the compressible Navier-Stokes-Korteweg system in the relaxation limit $\alpha \to \infty$ and $\beta \to 0$. In the first part of this talk, we introduce the class of finite energy weak solutions to the initial-boundary value problem of the relaxation system and derive a corresponding relative energy inequality. In the second part of this talk, we use the relative energy inequality as a tool to prove two new analytical results for the relaxation model. First, we prove for fixed relaxation parameters that the relaxation model satisfies the weak-strong uniqueness property in the class of finite energy weak solutions. Then, we consider the relaxation limit $\alpha \to \infty$ and $\beta \to 0$. More specifically, we show that a sequence of finite energy weak solutions converges in the relaxation limit to a classical solution of the compressible Navier-Stokes-Korteweg system in strong norms, provided such a solution exists. As a byproduct we identify a convergence rate for this relaxation limit.

**Two-time scale dynamics of a 2D rimming-flow equation**
Joussen, Juri (1); Lienstromberg, Christina (1); Velázquez, Juan J. L. (2)
*1: University of Stuttgart, Germany*
*2: University of Bonn, Germany*
14:20

A *rimming flow* is the flow of a fluid partially filling a rotating cylinder. We assume that the fluid forms a capillary-driven thin film coating the inner wall. Considering only a cross-section of the cylinder, we formally derive a closed fourth-order degenerate-parabolic evolution equation for the height of the liquid film from the Navier–Stokes equations by means of a lubrication approximation. Competing effects relevant to this equation are the cylinder rotation, surface tension, viscosity and gravity. We investigate the stability of positive steady states. We prove an approximation result showing that the equation exhibits dynamics on two distinct time scales. In the fast time scale, the fluid is transported

by the cylinder rotation. For the slow time scale we derive a governing system of ODEs.
This talk is based on joint work with Christina Lienstromberg (Stuttgart) and Juan J. L. Velázquez (Bonn).

**Dynamics of a 3d rimming flow**
Lienstromberg, Christina (1); Joussen, Juri (1); Laudien, Janne (1); Velázquez, Juan (2)
*1: University of Stuttgart, Germany*
*2: Bonn University, Germany*
14:40

We study the dynamic behaviour of a thin viscous fluid film coating the inner wall of a rotating cylinder - a so-called *rimming flow*.
The resulting PDE for the height h > 0 of the fluid film is quasilinear, degenerate parabolic and of fourth order.
Various competing effects drive the dynamics of the interface - viscosity, surface tension and gravity. For a positive surface tension parameter $\gamma$> 0 of order one we investigate existence and stability of positive steady states, depending on the influence of gravity.

The talk is based on joint works with Juri Joussen (Stuttgart), Janne Laudien (Stuttgart) and Juan Velázquez (Bonn).

**A functionalized-Cahn–Hilliard type model for two-phase flow with surfactants**
Metzger, Stefan; Ullrich, Clemens
*Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*
15:00

The surface tension of a fluid interface can be reduced due to the presence of a surfactant (= 'surface active agent'). Surfactants are used in various industrial applications, e.g. as emulsifiers, detergents, or wetting agents. In this talk, we investigate a phase-field model for two-phase flow of incompressible fluids with surfactants.

The free energy governing the evolution incorporates a Cahn–Hilliard energy weighted by a (not necessarily nonnegative) prefactor that depends on the surfactant density, and a bending energy for the interface. As a result, an increase in interfacial area may be energetically favorable. This free energy functional resembles a functionalized Cahn–Hilliard energy, thus giving rise to a sixth-order Cahn–Hilliard–Willmore type equation for the phase-field parameter. Mathematical challenges are posed by the low regularity of the surfactant density.

We prove the existence of weak solutions on arbitrary time intervals, assuming the surfactant to be insoluble and the two fluids to be shear-thickening generalized Newtonian of power-law type. The argument is based on a semi-implicit discretization and a solenoidal Lipschitz truncation technique to deal with the nonlinearity in the viscous stress tensor.

**Short- and long-time behavior in evolution equations: the role of the hypocoercivity index**
Arnold, Anton
*TU Wien, Austria*
15:20

The "index of hypocoercivity" is defined via a coercivity-type estimate for the self-adjoint/skew-adjoint parts of the generator, and it quantifies 'how degenerate' a hypocoercive evolution equation is, both for ODEs and for evolutions equations in a Hilbert space. We show that this index characterizes the polynomial decay of the propagator norm for short time and illustrate these concepts for the Lorentz kinetic equation on a torus.
Discrete time analogues of the above systems (obtained via the mid-point rule) are contractive, but typically not strictly contractive. For this setting we introduce "hypocontractivity" and an "index of hypocontractivity" and discuss their close connection to the continuous time evolution equations.
This talk is based on joint work with F. Achleitner, E. Carlen, E. Nigsch, and V. Mehrmann.
References:
1) F. Achleitner, A. Arnold, E. Carlen, The Hypocoercivity Index for the short time behavior of linear time-invariant ODE systems, J. of Differential Equations (2023).
2) A. Arnold, B. Signorello, Optimal non-symmetric Fokker-Planck equation for the convergence to a

given equilibrium, Kinetic and Related Models (2022).
3) F. Achleitner, A. Arnold, V. Mehrmann, E. Nigsch, Hypocoercivity in Hilbert spaces, J. of Functional Analysis (2025).

## S15: Uncertainty quantification

Organizer(s): Sprungk, Björn *(TU Bergakademie Freiberg)*
Scarabosio, Laura *(Radboud University)*

## S15.01: Uncertainty-aware Optimization

Date: March 17, 2026 08:30–10:30
Room: KII, M17.21

### Shape optimization under uncertainty

Dambrine, Marc (1); Harbrecht, Helmut (2); Viacheslav, Karnaev (2) 08:30
*1: University of Pau, France*
*2: University of Basel, Switzerland*

This presentation aims to provide an overview of shape optimization under random loadings. Besides the minimization of the expected objective, we also consider the minimization of failure probabilities. We show that in these situations the objective and its gradient are explicitly determined by low-order moments of the random loading. We then derive cheap, deterministic algorithms to minimize the objective. Several applications and numerical compuations are given.

### Trust-Region Bayesian Optimisation with Local-Global Competition

Nobile, Fabio (1); Van Dieren, Eliott (1); Vanzan, Tommaso (2) 09:10
*1: EPFL, Switzerland*
*2: Politecnico di Torino, Italy*

Bayesian Optimisation (BO) has become a technique of choice for optimising expensive-to-evaluate functions under a limited computational budget. However, standard BO relies on a global acquisition function to guide the sampling of new candidates, which may hinder the exploitation of promising regions around potential minimisers. Furthermore, oversampling in promising regions can lead to the ill-conditioning of the Gaussian Process (GP), which serves as the surrogate model in BO.

In this work, we introduce a novel local-global framework that combines trust-region methods with BO via a competition mechanism. At each iteration, both techniques propose a candidate, and a selection criterion determines which one is accepted. This approach alleviates both the poor local refinement and the ill-conditioning of the conventional BO method when reaching the promising area of a local optimum, while still preserving a global surrogate. As a result, the method allows for a better exploration of the full design space compared to standard non-linear optimisation algorithms for smooth functions.

The technique employs gradient-enhanced GPs for the global surrogates and quadratic models for the local trust-region exploitation. It is hence particularly well-suited for optimisation tasks involving expensive-to-evaluate non-convex functions with available gradients. The efficacy of the proposed method is supported by a comparison against state-of-the-art optimisation routines on challenging synthetic problems, as well as an application to PDE-constrained optimisation.

### Robust design optimization using semi-intrusive Taylor series approximations of different order

Kriegesmann, Benedikt; Krüger, Jan 09:30
*Technische Universität Hamburg, Germany*

Design optimization of structures tends to provide designs which are sensitive to deviations from the ideal configuration, for which they are designed. Robust design optimization approaches allow for taking into account the influences of randomly scattering material properties, geometry and loads. A typical optimization formulation includes the mean and variance of some response function of interest in the optimization objective. When using gradient-based optimization algorithms, not only these stochastic moments but also their gradients need to be determined as efficiently as possible. One

class of approaches, that is presented in the current talk, approximates the response function with Taylor series expansions with respect to the random parameters.

When using first-order expansions, the computational cost per optimization iteration increases only by a factor of two to four [1,2], independently of the number of random parameters considered. This comes at the cost of low accuracy and for certain applications, first-order approaches fail to provide a robust design. Second-order approximations cover a wider range of applications. However, the computational cost per optimization iteration scales at least linearly with the number of random parameters [3].

The reason for the increased cost originates from the determination of higher-order derivatives of the response function with respect to random parameters. All required derivatives are determined by the adjoint method. However, the memory may become extreme [1] and in some cases, such as eigenvalue minimization problems, the adjoint systems cannot be solved [2]. This is circumvented by using semi-intrusive approximations [2,3], which will be presented.

For some applications in structural optimization, in particular buckling-prone problems, the response function may be discontinuous, leading to a multimodal output distribution [4]. For such problems, all approximations based on local expansions fail. Therefore, a method is presented that combines local expansions in different regions of the random space and therefore allows to applying efficient Taylor expansion-based approaches also to these types of problems.

[1] Kranz, Lüdeker, Kriegesmann. „A Generalized Approach for Robust Topology Optimization Using the First-Order Second-Moment Method for Arbitrary Response Functions". *SMO* (2023) https://doi.org/10.1007/s00158-023-03540-w.

[2] Krüger, Kranz, Schmidt, Seifried, Kriegesmann. „An Efficient and Non-Intrusive Approach for Robust Design Optimization with the First-Order Second-Moment Method". *CMAME* (2023) https://doi.org/10.1016/j.cma.2023.116136.

[3] Krüger, Kriegesmann. „Robust Design Optimization Using a Non-Intrusive Second-Order Approximation of Stochastic Moments". *SMO* (2024) https://doi.org/10.1007/s00158-024-03843-6.

[4] Kriegesmann, Krüger, Steltner, Schmidt, Seifried. „Robust Design Optimization of Structures with Multimodal Responses Using Taylor Expansions". *SMO* (2025) https://doi.org/10.1007/s00158-025-04191-9.

**Risk sharing and belief distributions in systems with uncertainty of physical properties and human actions**

Pettersson, Per (1); Krumscheid, Sebastian (2); Tveit, Svenn (1); Gasda, Sarah (1) 09:50
*1: NORCE Norwegian Research Centre, Norway*
*2: Karlsruhe Institute of Technology, Germany*

We consider cooperative game models where otherwise independent agents acting on a technical system with uncertainty in its response can choose to form coalitions for collaboration. Each coalition acts as a single entity and will obtain a value or payoff determined by the response of the technical system. Each agent is faced with the decision problem whether to join a given coalition or not, and, if they do join, how the payoff should be distributed among the coalition members. The payoffs are stochastic, and the decision making is ultimately a choice between different random variables. While there is no single natural way to choose between random variables, different so-called preference relations can be used to systematically make a direct comparison.

The technical system that determines the agents' payoffs can be described by a computational model whose response depends on both physical parameters, and the actions of the agents. Uncertainty in the physical parameters can be modeled by random variables and fields, and their effect on some system quantity of interest can be estimated by forward uncertainty propagation through the model, using e.g. accelerated Monte Carlo simulation.

In the situation that the agents cannot affect each other at all via actions on the system, coalition formation and stochastic preferences are still relevant as they provide a means to perform risk sharing, much like an insurance system.

When the agents are in the position to affect the possible payoffs for other agents by their actions on the system, the situation is further complicated. While the physical properties can be treated with probabilistic models, at least if there are data to support them, it is not straightforward to model unknown human action by random variables. We propose belief distributions for unknown human action based on the idea that the stochastic model should be as un-informative as possible, while using as much physical information as possible. In this manner, we strive to avoid a false sense of knowledge by avoiding assumptions not supported by data and simultaneously make the model as true to actual data as possible.

The ideas are illustrated by numerical results from realistic cases of permanent CO2 storage. We discuss prospects and challenges related to 1) modelling and representation of belief distributions, 2) efficient propagation of belief distributions and physical uncertainties to quantities needed for decision making, and 3) decision making under uncertainty from a risk sharing perspective.

**New formulation for process-based global sensitivity indices**

Kohlhaas, Rebecca (1); Ceresa, Laura (2,3); Guadagnini, Alberto (3); Riva, Monica (3) 10:10

*1: University of Stuttgart, Germany*
*2: Universitat Politecnica de Catalunya, Spain*
*3: Politecnico di Milano, Italy*

Process-based modeling across a broad spectrum of physical, chemical, and engineering systems is inherently subject to substantial uncertainty, arising from process conceptualization and the estimation of uncertain model parameters. Hence, the development of robust and quantitative metrics to assess the sensitivity of model outputs to alternative process representations and parameter choices is a critical component of several disciplines, encompassing, e.g., hydrology, environmental engineering, and geosciences. Within a stochastic modeling framework, systematic evaluation of the contribution of individual processes to system behavior, together with rigorous quantification of the uncertainty associated with their implementation and level of parameterization, enables a coherent mathematical representation of our conceptual understanding of the underlying system dynamics.
In this context, uncertainty and sensitivity associated with process representation can be systematically explored by constructing ensembles of models that incorporate alternative process formulations. Rigorous analysis and uncertainty quantification for such model ensembles require extensions of existing methodologies to explicitly condition on process choices in addition to parameter variability. Global sensitivity analysis plays a central role in this sense, as it enables quantitative assessment of the influence of both process-related parameters and process formulations on model outputs. Accordingly, extensions of established sensitivity measures (most notably variance-based Sobol' indices and moment-based AMA indices) have been developed to explicitly account for process-level sensitivity.

Here, we focus on process-related AMA sensitivity indices and introduce a new family of formulations designed to complement their original counterparts and to provide enhanced insights into process sensitivity. In contrast to existing formulations, which attribute uncertainty contributions to individual models within the ensamble, the new indices adopt a process-centered perspective. This shift allows direct quantification of the impact of individual process formulations on the variability of key statistical moments of a quantity of interest.
We conduct a detailed and rigorous theoretical analysis of both the original and proposed indices to elucidate their conceptual distinctions and to clarify the interpretation of differences in their respective values. The two sets of indices are then applied and compared across three scenarios spanning increasing levels of model complexity. Our results demonstrate that the proposed indices yield additional and complementary understanding of the way process formulations and their associated (uncertain) parameters influence model behavior and contribute to shape model output uncertainty.

**S15.02: Forward Uncertainty Quantification: Modeling and Approximation**
Date: March 17, 2026 16:30–18:30
Room: KII, M17.21

**An adaptive sparse Galerkin FEM for the log-transformed diffusion problem**

Eigel, Martin; Merdon, Christian
*WIAS, Germany*

16:30

Adaptive sparse polynomial chaos discretisations for parametric random PDEs within the stochastic FEM framework have been studied for more than a decade. Recent work has established convergence and (instance-)optimality results, thereby closing several gaps relative to classical FEM theory. These results, however, typically assume an affine dependence of the coefficient on a countably infinite set of parameters, which excludes the more challenging lognormal case, one of the principal settings in which Monte Carlo methods remain predominant.

In this work, we revisit the log-transformation used by Ullmann, Elman, and Ernst (2012) and develop a residual-based a posteriori error estimator to drive adaptive refinement. The transformation yields a convenient reformulation of the lognormal diffusion problem as a convection–diffusion equation with affine parametric dependence. A key difficulty is to relate the residual of the transformed problem to the error measured in the natural norm of the original formulation. We address this by establishing an equivalence in an appropriate dual norm and present numerical experiments demonstrating the favourable practical performance of the resulting adaptive method.

**Gevrey regularity for lognormal diffusion problem with non-linear parameterization**

Chernov, Alexey (1); Dũng, Đinh (2); Lê, Tùng (1)
*1: University Oldenburg, Germany*
*2: Information Technology Institute, Vietnam National University, Hanoi, Vietnam*

16:50

We study the parametric regularity of solutions to linear, elliptic partial differential equations in divergence form. The main challenge lies in problems with countably-parametric inputs, specifically focusing on challenging cases where the diffusion coefficient exhibits singularities or has a non-compact support, such as those modeled by Gevrey-class functions or log-normal distributions. To address this, we employ the falling-factorial technique, which serves as a powerful tool for proving the regularity of solutions with respect to their parameters. This work has significant applications for numerical analysis, providing a robust framework for proving the convergence of numerical methods like Gaussian quadrature and quasi-Monte Carlo integration.

**Surrogate Based Uncertainty Quantification for Large-Scale Vibroacoustics**

Eßling, Robin (1); Römer, Ulrich (1); Büsing, Aaron (2); Bollhöfer, Matthias (2)
*1: TU Braunschweig, Germany (Institut für Akustik und Dynamik)*
*2: TU Braunschweig, Germany (Institut für numerische Mathematik)*

17:10

This work presents a surrogate modeling strategy for uncertainty quantification in large-scale vibroacoustic systems. In these systems, parameters such as Young's modulus or material thickness are uncertain due to the manufacturing process or lack of knowledge. As a result, computing statistical moments of quantities of interest - such as expected sound pressure levels - requires solving the underlying system thousands of times, which is computationally infeasible. This challenge becomes even more severe when the frequency-dependent pressure response must be evaluated over a wide frequency band.

In order to obtain an accurate surrogate model, we consider projection based reduced order modeling, where the projection matrix is constructed via multi-moment-matching. While this approach can yield sufficiently accurate surrogates for only a few parameters, it becomes computationally expensive in high-dimensional settings due to the large number of resulting multi-moments.

To manage this, a predefined number of expansion points for multi-moment-matching is selected using an adaptive sparse grid approach. The global projection matrix is constructed using only zeroth- and first-order moments, which serve as an error indicator. By matching only the most sensitive moments at each expansion point – identified through a local error estimator and local sparse index set - a sparse global projection basis can be obtained. This approach yields a global projection matrix of moderate dimension with acceptable approximation errors especially in cases where the number

of stored LU decompositions is limited. The method will be illustrated with numerical results on the two-dimensional Helmholtz equation with varying numbers of uncertain input parameters.

**Uncertainty Quantification for Nonlocal Traffic Flow using stochastic Galerkin approximations**

Ziegler, Fabian; Göttlich, Simone
*Universität Mannheim, Germany*

17:30

Nonlocal Traffic Flow models have been introduced to model macroscopically the effect of downstream information on the behaviour of drivers. The term 'nonlocal' refers to the dependence of the flux function on a convolution term between a kernel function and the conserved quantity. However, in the real world one needs to account for additional uncertainties in the model such as measurement errors or uncertainty in the drivers' behaviour. Thus, the distribution of vehicles depends additionally on some random input.

The idea to represent such stochastic processes by orthogonal polynomials has been employed in uncertainty quantification and inverse problems for other problems. This approach is known as stochastic Galerkin formulation with a generalized polynomial chaos (gPC) expansion. The gPC expansions of the stochastic input are substituted into the governing equations. An important benefit of polynomial chaos methods is that they exhibit spectral convergence, leading to high accuracy with relatively few expansion terms. However, these approaches can fail in the case of flows involving discontinuities with respect to the random variables. Instead one can use stochastic collocation methods which are non-intrusive and use a deterministic approximation for the Galerkin modes just as in Monte–Carlo based methods. Another problem is posed by the fact that the deterministic Jacobian of the projected system differs from the random Jacobian of the original system and hence hyperbolicity is not guaranteed.

It can be shown that for flux functions, linear with respect to the convolution, and a suitable polynomial basis, the hyperbolicity for the nonlocal traffic flow model is preserved. Furthermore, spectral convergence is observed and the numerical results agree with the results obtained by stochastic collocation and Monte-Carlo sampling.

**Stochastic modeling of local variations in packaging paper via spatial random fields**

Pfeifer, Jan Mirco (1); Hirn, Ulrich (2); Neumann, Johannes (1); Simon, Jaan-Willem (1)
*1: University of Wuppertal, Germany*
*2: Graz University of Technology, Austria*

17:50

The transition toward sustainable materials in construction and engineering has renewed interest in paper as an eco-friendly resource. Realizing this opportunity, however, requires a more comprehensive understanding of its mechanical properties.

Paper, as a fibrous material, is heterogeneous due to inherent local variations in basis weight (grammage), thickness, and fiber orientation. This spatial variability introduces substantial uncertainty in predicting its mechanical response. We address this by developing a stochastic modeling approach that synthesizes local variations through spatial random fields.

The aim of this contribution is to characterize the variability in packaging paper through spatial analysis and to develop a framework for synthesizing this variability using stochastic models. By analyzing and reproducing the statistical properties of observed spatial variations, we enable systematic exploration of local heterogeneity without sole dependence on experimental measurements.

Our methodology comprised four key steps. First, we performed semivariogram analysis of experimental maps of local variations to quantify spatial correlations. Second, we fitted a parametric semivariogram model to the analyzed data. Third, we generated multiple spatial random field realizations using the fitted semivariogram model to capture the statistical and spatial characteristics of real packaging paper. Fourth, we validated the generated realizations to ensure they accurately reproduce the observed spatial properties.

By establishing a parametric framework for local variations, this work reduces reliance on physical measurements and provides a versatile foundation for uncertainty quantification. The approach enables systematic investigation of how spatial heterogeneity influences mechanical response in packaging paper and other fibrous materials. This contribution bridges spatial statistics and stochastic modeling, offering practical tools for uncertainty quantification in computational mechanics of heterogeneous materials.

**Positive random fields without exponential transformation as coefficients in the stochastic diffusion equation**

Gottschalk, Hanno 18:10
*TU Berlin, Germany*

Usually the uncertainty in the coefficients of the stochastic diffusion equation is modeled with log-Gaussian randomfields, i.e. Gaussian random fields are exponentiated to reneder them positive. Recently, it has been proposed to replace Gaussian random fields with log-Lévy random fields and then proceed as in the Gaussian case. In this talk I show that for Lévy random fields with inifinite activity and positive Lévy measure, however without a Gaussian or deterministic contribution, the existence of (pathwise) solutions can be obtained in an almost sure sense and in addition the existence on moments can be derived as well. While in the case with exponentiatiation, the extremal value theory for Gaussian and Lévy random fields has to be employed (on the positive and nehative side), for the non exponentiated version we require a minimum value theory. This can be derved from the minimum value assumption. The talk is based on joint work with Sebasian Kohlmann.

## S15.03: Uncertainty Quantification in Engineering and Societal Applications

Date: March 18, 2026 08:30–09:30
Room: KII, M17.21

**Prioritising Barriers to Sustainable Humanitarian Logistics Operations Using the Fuzzy Best–Worst Method: Evidence from NGOs Operating in Gaziantep, Türkiye**

Özceylan, Ayca (1); Tanyaş, Mehmet (2) 08:30
*1: Gaziantep University, Turkey (Türkiye)*
*2: Maltepe University, Turkey (Türkiye)*

Sustainable humanitarian logistics is increasingly emphasised by donors and practitioners, yet implementation remains challenging—especially in protracted crises where speed, equity, accountability, and cost pressures can conflict with environmental and long-term socio-economic goals. This study aims to identify the key barriers that hinder sustainable humanitarian logistics operations and to prioritise them by reflecting the uncertainty inherent in expert judgements. First, a comprehensive "barrier pool" is compiled through a structured review of relevant peer-reviewed studies published over the last ten years, complemented with evidence from NGO and humanitarian-sector reports to ensure practical relevance. The resulting candidate barriers are consolidated, refined, and grouped under the triple-bottom-line dimensions of sustainability (economic, social, and environmental).

Second, the study collects assessments from subject-matter experts working in NGOs that are actively operating in Gaziantep, Türkiye—an important humanitarian coordination and operations hub. To capture ambiguity in experts' linguistic evaluations (e.g., "high", "very high", "moderate") and to obtain consistent priorities with a limited number of pairwise comparisons, the Fuzzy Best–Worst Method (F-BWM) is employed. Experts identify the best (most critical) and worst (least critical) barriers within each dimension and provide fuzzy comparisons, which are then transformed into weights and rankings via an optimisation-based procedure. The ranked barriers are further clustered into actionable themes to support managerial interpretation.

The findings reveal that the most critical economic barrier is inadequate and volatile funding, which restricts life-cycle cost thinking, sustainable procurement choices, and investments in greener assets and transport. The most critical social barrier is limited human capacity and sustainability competence, evidenced by staff turnover, insufficient training, and weak institutionalisation of sustainability

routines across partners. The most critical environmental barrier is limited access to low-emission logistics options and enabling infrastructure (e.g., cleaner transport alternatives, energy-efficient warehousing, and effective waste/reverse-logistics arrangements). Overall, the study provides a context-grounded prioritisation to guide NGOs and donors toward high-leverage interventions for sustainable humanitarian logistics.

**Quantifying Model Form Uncertainty, Influence and Separability in Data-driven Calibration of Tendon Break Models**

Andrés Arcones, Daniel (1,2); Paul, Aeneas (3); Weiser, Martin (4); Sanio, David (3); Unger, Jörg F. (1) 08:50
*1: Bundesanstalt für Materialforschung und -prüfung, Germany*
*2: Technical University of Munich, Germany*
*3: Ruhr University Bochum, Germany*
*4: Zuse Institute Berlin, Germany*

Fiber optic sensors (FOS) are increasingly used for structural health monitoring of bridges, providing dense and distributed strain measurements. An especially relevant application is the detection and localization of tendon breaks, where not only the occurrence but also the depth of the damaged tendon must be identified. To explore this possibility, an experimental setup was established to reproduce the boundary and loading conditions of a bridge tendon, and FOS strain observations were collected during controlled failure events. A finite element (FE) model of this experiment was developed and is used here as a gray-box simulator. Its parameters are calibrated against the FOS data, and the resulting probabilistic characterization is transferred to more realistic models in which different tendon depths are simulated and compared to observed deformation fields.

Because of the complexity of the tendon break phenomenon, model form uncertainty (MFU) plays a decisive role. Bayesian calibration is performed while explicitly accounting for MFU through an embedded representation in which a prescribed set of parameters captures the model–reality discrepancy. This formulation enables the quantified MFU to be consistently propagated to other models and quantities of interest. Due to the computational cost of FE simulations, Gaussian Process surrogates are employed, and their predictive uncertainty is incorporated into the calibration to ensure coherent uncertainty propagation.

The calibration reveals that some observations cannot be represented by any admissible parameter values, indicating structural model inadequacies. To identify and characterize these, an influence analysis of the observations on the posterior distribution is carried out. The $\varphi$-divergence between posterior distributions with and without individual observations is evaluated to quantify their impact on the calibrated posterior. Furthermore, by examining the influence on the marginal posterior components within the embedded MFU formulation, it becomes possible to determine which observations drive the parameters associated with model discrepancy and which parameters are most affected, guiding model refinement and experimental design.

Finally, when the calibrated parameters are transferred to alternative models, the separability of predictions for different tendon depths is analyzed. The overlap between predictive distributions is quantified to determine the minimum resolvable depth difference and regions of non-separability arising from MFU. This analysis defines the achievable resolution for tendon break localization and informs optimal sensor placement strategies under uncertainty.

**Simulation of thermo-viscoelastic structures under material uncertainties using Time-separated Stochastic Mechanics**

Müller, Christian; Geisler, Hendrik; Junker, Philipp 09:10
*Leibniz University Hannover, Institute of Continuum Mechanics, Hannover, Germany*

Time-separated Stochastic Mechanics (TSM) provides a new methodology to take randomness in material models into account. Numerical costs of uncertainty quantification are heavily reduced compared to classical methods. The TSM is based on a Taylor series of all field variables, i.e. displacement and internal variable, in the random variables. This leads to a separation of the random time independent behavior from the deterministic time dependent behavior. For each random variable only

a single additional system of equations has to be solved. This can be done efficiently with standard finite element software. The efficiency and accuracy of TSM for uncertainty quantification of a variety of inelastic materials and structures has been shown in [1], [2]. TSM results are typically nearly indistinguishable from reference Monte Carlo simulations. In this talk, we present the extension of TSM for structures with a thermo-viscoelastic material model. Due to the heat diffusion, the problem is non-local in nature. For the first time, we present the application of TSM to non-local inelastic problems. All fields, e.g., temperature field and stress field are random due to the random material parameters as Young's modulus and coefficient of thermal expansion. Evaluating the expectation and standard deviation of the quantity of interest, e.g., the stress field. The quantification of efficiency and accuracy is done by comparison to reference Monte Carlo simulations.

References

[1] H. Geisler and P. Junker. "Time-separated stochastic mechanics for the simulation of viscoelastic structures with local random material fluctuations". en. In: Computer Methods in Applied Mechanics and Engineering 407 (Mar. 2023), p. 115916. issn: 00457825. doi: 10.1016/j.cma.2023.115916.

[2] H. Geisler, C. Erdogan, J. Nagel, and P. Junker. "A new paradigm for the efficient inclusion of stochasticity in engineering simulations: Time-separated stochastic mechanics". en. In: Computational Mechanics (July 2024). issn: 0178-7675, 1432-0924. doi: 10.1007/s00466- 024-02500-5.

## S15.04: Bayesian Estimation and Filtering

Date: March 18, 2026 14:00–16:00
Room: KII, M17.21

### Filtering with Randomised Observations: Sequential Learning of Relevant Subspace Properties and Accuracy Analysis

de Wiljes, Jana (1); Dubinkina, Svetlana (2); Abedini, Nazanin (2) 14:00
*1: TU Ilmenau, Germany*
*2: VU Amsterdam*

Merging data and models to estimate the current states and parameters of a system of interest is essential for modern decision-making and planning across many applications related to societal issues. Depending on the complexity and nature of the problem, different classes of filtering methods are employed to address this task. The family of Ensemble Square Root Filters (ESRFs) is widely used across various application areas due to their computational efficiency, robustness, and capability to track signals in nonlinear and high-dimensional settings. Many of these discrete filters are connected, in the time-continuum limit, to a deterministic version of the Ensemble Kalman-Bucy Filter (EnKBF). Recently, the long-term stability and accuracy of this continuous EnKBF family were investigated under idealized conditions, assuming the underlying system was fully observed. It is possible to derive similar results for specific model classes and to utilize the respective properties of the associated systems. In this study, we examine the signal processing capabilities of the filter under fixed, randomized, and adaptively changing partial observations. We establish bounds on the expected signal-tracking performance relative to the underlying random measurements and introduce a sequential algorithm that adaptively learns an optimal size of the state-space subset. Such an adaptive method can be used to gain a better understanding of underlying systems and serves as a sequential heuristic tool to identify and focus on size of the most relevant subspace of the state space.

### Numerical Inference for the Porous Medium Equation

Blessing, Lea; Hornischer, Niklas; Barth, Andrea; Göddeke, Dominik 14:40
*University of Stuttgart, Germany*

Inverse problems for nonlinear diffusion equations aim to infer a system's properties from limited observations of its evolution, rendering them an important tool in various fields such as geophysics and medical imaging. As these problems are inherently ill posed due to measurement noise, a major challenge is to develop robust and efficient methods for uncertainty quantification. We focus on parameter inference for the porous medium equation (PME) which is particularly challenging, being

a nonlinear degenerate parabolic equation. Understanding the medium's properties is crucial in applications such as groundwater modelling or simulating drug delivery in tissues. To recover these parameters, observations may be available at discrete spatial locations over time which reflects realistic measurement constraints. We employ Bayesian inversion which allows us to incorporate measurement noise, as well as prior information into our model. In this setting, we examine the theoretical properties of the posterior, which represents the inverse problem's solution, including the problem's well-posedness. A main contribution is the reformulation of the inverse problem in a way that exploits the structure of the PME, leading to an auxiliary elliptic inverse problem that may be solved instead. This allows us to formulate an efficient numerical method for solving the inverse problem which has mainly been discussed in theory so far. We present numerical experiments, demonstrating the computational performance of the proposed method in practice.

**Low-rank approximations for linear Gaussian inverse problems in infinite dimensions**

Carere, Giuseppe; Lie, Han Cheng
*University of Potsdam, Germany*

15:00

Computationally efficient low-rank approximations of linear Gaussian inverse problems enable the tractable estimation of high-dimensional parameters. However, the analysis of their optimality properties has so far been restricted to parameter spaces of a fixed, finite dimension, which can for instance arise from a discretised PDE. In this talk, we study the low-rank approximation of linear Gaussian inverse problems in infinite dimensions. We develop a theoretical framework for efficiently approximating the Gaussian posterior mean and covariance, by solving variational low-rank approximation problems for Gaussian measures on Hilbert spaces. Our results are inherently discretisation-independent and reveal structural properties of the low-rank posterior approximation procedure that are obscured after discretisation.

**Bayesian estimation of multiphase properties from images of holes in liquid films**

Bonart, Henning
*Technische Universität Darmstadt, Fachbereich Maschinenbau, Germany*

15:20

Accurate measurement of interfacial properties in multiphase systems is critical for process control in manufacturing and for advancing our understanding of fluid dynamics and materials science. However, key parameters such as surface tension and contact angles are often difficult, costly, or slow to measure directly, particularly in situ without disturbing the process. We present a novel model-based approach for measuring multiphase properties and their uncertainties from simple optical images of thin liquid film defects. Our method fuses images captured with a standard camera with a physics-based model of film dynamics in a Bayesian framework. This enables simultaneous estimation of multiple geometric and physical parameters, including surface tension, substrate contact angle, and film thickness, along with rigorous uncertainty quantification. In this talk, we present the derivation and implementation of the full Bayesian inverse problem, including the governing physics and practical approximation strategies for computational efficiency. We then demonstrate the effectiveness of our approach on real experimental data, showing that accurate parameter estimation can be achieved from readily available imaging equipment without specialized instrumentation or process interruption.

**Nonasymptotic subsampling rate identification for parameter estimation of SDEs in multi-scale scenarios**

Trolldenier, Felipe (1); Lindner, Felix (1); Schmeißer, Andre (2); Wegener, Raimund (3)
*1: University of Kassel*
*2: Fraunhofer ITWM Kaiserslautern*
*3: private*

15:40

In many practical applications, models based on stochastic differential equations (SDEs) fail to accurately represent available data at small scales. As a consequence, classical approaches to parameter estimation in SDEs - such as diffusion coefficient identification based on the quadratic variation of

the path - exhibit a bias if the data are not subsampled. Since the optimal subsampling rate is generally unknown, we introduce a method for selecting suitable subsampling rates, based on counting the lengths of consecutive increments with identical signs, which we refer to as monotone runs. The theoretical foundation of our method relies on results concerning the distribution of monotone-run lengths at the infinitesimal scale of the underlying SDE model. Assuming ergodicity, the mean length of monotone runs along a path provides a consistent approximation of the corresponding expected value derived from the model. Suitable subsampling rates can therefore be identified by comparing the empirical mean length of the monotone runs in the data in dependence on the subsampling rate with the theoretical expected value. This method is directly applicable to data and does not rely on asymptotic assumptions associated with multiscale settings such as homogenization. We demonstrate the approach using a stochastic model for the efficient simulation of fiber lay-down processes in industrial production processes of nonwoven textiles. In this context, we perform numerical tests using simulated data in a homogenization setting as well as applications to real-world data.

## S15.05: Computational Methods for Efficient Bayesian Inference

Date: March 18, 2026 16:30–18:30
Room: KII, M17.21

### Distributed Multilevel Sequential Monte Carlo Applied to PDE-Based Bayesian Inverse Problems

Baumgarten, Niklas 16:30
*Heidelberg University, Germany*

We present a distributed multilevel sequential Monte Carlo method for Bayesian inverse problems to identify high-dimensional
input parameters of models based on partial differential equations. The method is implemented on a distributed multilevel data structure
to divide the computational load across multiple processing devices and to control the sampling and discretization errors introduced
by Monte Carlo estimation and finite element approximation. By formulating these errors as the minimization target in a knapsack problem,
with available computational resources as constraints, we derive error bounds with respect to a given computational budget.
Based on this framework, we discuss convergence properties and present experimental results demonstrating the method's performance.

### A Laplace Mixture Method for Multimodal Bayesian Inference

Egéa, Maxime (2); Gu, Hanyue (1); Rudolf, Daniel (3); Sprungk, Björn (1) 16:50
*1: TU Bergakademie Freiberg*
*2: Sorbonne Universite*
*3: University of Passau*

In Bayesian inference, accurately approximating the posterior distribution is essential for deriving meaningful probabilistic insights from data. The Laplace approximation provides a computationally efficient Gaussian approximation of posterior distributions in Bayesian inference. However, its accuracy deteriorates for complex posteriors, such as those exhibiting multimodality or strong non-Gaussianity. To address this, we introduce a method that constructs a proposal distribution as a convex mixture of local Laplace approximations. We prove the theoretical convergence of this Laplace-Mixture towards the target posterior, establishing a bound on the Hellinger distance as observational noise diminishes. Our primary contributions are twofold: first, we provide a theoretical analysis of its performance in Monte Carlo methods, proving the convergence of the Effective Sample Size (ESS) in Importance Sampling and of the acceptance rate and Expected Squared Jumping Distance (ESJD) in Independent Metropolis-Hastings. Second, we demonstrate through numerical examples that our method remains robust and efficient as the number of observations increases and the observational noise decreases, validating our theoretical results.

**Markov Chain Monte Carlo for Particle Solvers**

Løvbak, Emil; Krumscheid, Sebastian
*Karlsruhe Institute of Technology, Germany*

17:10

In various application domains, one wishes to determine which parameter values should be used for a model to match its simulation output with measurement data. In practice however, measurement error on the data means that, at best, one can produce a so-called posterior probability distribution of these parameter values, given an assumed noise model. The Markov chain Monte Carlo method is a popular approach that constructs a Markov chain with this posterior distribution as its invariant distribution. The parameter samples in the chain are selected through an accept-reject strategy, that accepts proposal samples, based on their likelihood, relative to that of the previous accepted sample.

Evaluating this likelihood requires the solution of the given model. Therefore, any errors in the discrete solver will result in errors in the likelihood evaluation. In this presentation, we discuss the case where the Markov chain Monte Carlo method is run on top of a stochastic solver, such as a Monte Carlo particle solver. In this case, the likelihood — and thus the acceptance probability — becomes a random variable who's variance scales with the number of random trajectories simulated by the solver. We discuss the mismatch between theory and practice in this setting. To this end, we combine classical error analysis and simulation results to understand the behavior of the pseudomarginal Markov chains in this setting. We then present practical approaches for efficient estimation in such settings.

**Slice Sampling Using Approximations**

Bitterlich, Kevin (1); Rudolf, Daniel (2); Sprungk, Björn (1)
*1: TU Bergakademie Freiberg, Germany*
*2: U Passau, Germany*

17:30

Slice sampling is a well-established Markov chain Monte Carlo (MCMC) method for drawing approximate samples from a posterior distribution that is often known only up to a normalizing constant. The method is based on choosing a new state on a slice, i.e., a superlevel set of the (unnormalized) target density with respect to a reference measure. However, slice sampling algorithms typically require multiple evaluations of the target density per iteration and can therefore become computationally expensive, particularly in high-dimensional settings. To mitigate these costs, in this talk we examine how deterministic approximations of the target density can be incorporated into slice sampling schemes. We demonstrate the effectiveness of our methods with several numerical experiments in the context of Bayesian inference.

**Experimental Design under Uncertainty**

Bartuska, Arved (4); Carlon, André (2); Espath, Luis (3); Hoang, Vinh (2); Krumscheid, Sebastian (1); Tempone, Raul (4)
*1: Karlsruhe Institute of Technology, Germany*
*2: RWTH Aachen, Germany*
*3: University of Nottingham, England*
*4: King Abdullah University of Science and Technology, Saudi Arabia*

17:50

Uncertainties are prevalent across various scientific and engineering fields, such as biomedical engineering, (financial) risk assessment, and materials science, where mathematical modeling and simulation play a central role. Accurately quantifying and reducing these uncertainties is crucial for reliable predictions and optimal system performance. Inverse problem formulations provide a rigorous framework for integrating noisy data with underlying models, yet acquiring sufficient data is often hindered by the high costs and time requirements of real-world experiments. Bayesian experimental design offers a principled strategy for assessing and optimizing experimental setups, thereby maximizing the value of limited data. However, its practical adoption is frequently hampered by substantial computational burdens, particularly the evaluation of nested integrals. This talk will present the core concepts of Bayesian experimental design and highlight recent advances in cost-effective approximation techniques, including hierarchical and projection-based methods, that address these

computational challenges, enabling efficient and practical experimental design in data-constrained environments.

## S15.06: Scientific Machine Learning for Uncertainty Quantification

Date: March 19, 2026 08:30–10:30
Room: KII, M17.21

### Generalized Gaussian process with equivariant neural operators

Liu, Zhuo-Ran (1); Zhou, Xu-Hui (2,3); Nowak, Wolfgang (1); Xiao, Heng (1) 08:30
*1: Stuttgart Center of Simulation Science, University of Stuttgart, Stuttgart, 70569, Germany*
*2: Scripps Institution of Oceanography, University of California San Diego, La Jolla, 92093, CA, USA*
*3: Computing + Mathematical Sciences, California Institute of Technology, Pasadena, 91125, CA, USA*

The Gaussian process provides a principled Bayesian framework for learning functions and quantifying uncertainty, but its practical use is often limited by restrictive kernel choices and limited expressive power. Deep neural networks, by contrast, can represent highly complex functions but typically lack calibrated uncertainty and a clear Bayesian interpretation. Bridging expressive modeling with fully Bayesian inference in a tractable and interpretable manner remains a fundamental challenge. In this work, we introduce the generalized Gaussian process, a fully Bayesian formulation that extends the classical Gaussian process by replacing fixed covariance kernels with a structured, operator-based representation. This framework preserves the probabilistic semantics of the Gaussian process while enforcing explicit mathematical constraints required for valid Bayesian inference. Rather than prescribing a specific kernel family, the covariance structure is learned through neural operators under these constraints, substantially expanding modeling flexibility beyond standard Gaussian process kernels. Hyperparameters within the learned covariance representation are treated using standard maximum a posteriori estimation, consistent with classical Gaussian process practice. We show that the generalized Gaussian process correctly degenerates to the classical Gaussian process in data-sparse regimes. As additional observations become available, the model adapts its covariance structure beyond fixed-kernel assumptions while maintaining fully Bayesian uncertainty propagation and well-calibrated predictive distributions. These properties are demonstrated through a set of carefully designed test cases. We consider structured synthetic examples that expose known limitations of the classical Gaussian process, including functions composed of multiple repeated but spatially varying local features, signals with sharp non-differentiable peaks that are oversmoothed by standard kernels, and functions exhibiting distinct correlation scales in different regions of the input domain. Overall, this work establishes the generalized Gaussian process as a principled and scalable extension of the Gaussian process, providing a robust foundation for uncertainty-aware modeling in data-efficient and scientific applications.

### Polymorphic Uncertainty Quantification of Composite Materials by Homogenization based on Physics-Augmented Neural Networks

Harazin, Felix; Platen, Jakob; Schietzold, F. Niklas; Graf, Wolfgang; Kaliske, Michael 08:50
*Technische Universität Dresden, Germany*

In the contribution at hand, it is aimed to incorporate and evaluate the uncertainty in multiscale uncertainty analyses. The realistic modeling of structures is fundamental for high-quality conclusions obtained from their numerical simulation. The effective material behavior of composite materials (e.g., concrete, spinoidal structures) is strongly affected by the heterogeneities occurring as a result of the combination of their individual components. Polymorphic uncertainty is a model used to describe variability and imprecision observed in databases and thus used for the realistic modeling of structures based on numerical mod els and the database at hand. If an engineering structure consisting of composite materials with inherent uncertainty is evaluated numerically, the combined quantification of uncertainty and composite material leads to computationally costly simulations. In order to handle the numerical effort, first, a scale separation is introduced to make the simulation complexity feasible. Thereby, the engineering structure is modeled at the macroscale, and the composite material is modeled by a Representative Volume Element (RVE) on the mesoscale. The RVE is evaluated by

a Finite Element (FE) scheme. Results on the macroscale are obtained by a nested FE scheme (FE2), where the RVE is used as a material model for the macroscopic FE analysis. While the numerical effort of the FE2 scheme is lower than without, the computational costs are still high. Secondly, to further reduce the numerical effort, Neural Networks (NN) are intro duced as surrogate models replacing RVE. NNs are a numerically efficient approximation scheme, while preserving accurate results, but large sets of numerically costly training data are required to train them. Thirdly, Physics-Augmented Neural Networks (PANN) are in troduced. Those incorporate physical properties in the architecture of the NN. By this, the required amount of training data is reduced. A framework is presented, which reduces the numerical effort of polymorphic uncer tainty quantification of composite materials. Consequently, the PANN is expanded with uncertain parameters to reduce the information required for PANN training. Therefore, a domain separation is proposed, which allows for efficient pre-training. A sampling scheme is presented, which enables the reduction of polymorphic uncertain input domains to a parametrized hypercube, based on the aleatoric and epistemic parts of the uncertainty model. The evaluation of aleatoric, epistemic, and polymorphic uncertainty from the mesoscale is evaluated at the macroscale by sampling over PANN, containing information about the modeled uncertainty.

**Uncertainty Quantification for Physics-Informed Neural Networks**

Späth, Henry (1); Gedikli, Talha (1); Varchev, Tihomir (2); Mandler, Hannes (3); Weigand, Bernhard (3); Staudacher, Stephan (2); Daw, Zamira (1)

*1: University of Stuttgart Institute of Aircraft Systems*
*2: University of Stuttgart Institute of Aircraft Propulsion Systems*
*3: University of Stuttgart Institute of Aerospace Thermodynamics*

09:10

Machine learning is becoming increasingly crucial in engineering as larger data sets and greater computational resources become available. One prominent application is the acceleration of costly simulations, often achieved by replacing conventional numerical solvers with data-driven surrogate models. Because physical laws govern most engineering problems, Physics-informed Neural Networks (PINNs) have emerged as a hybrid approach that embeds governing equations directly into the training loss. While numerous studies report that PINNs outperform classical feed-forward networks in terms of stability and generalization for the specific physical regime they are trained on, it remains unclear how they behave under parameter shifts or scenario changes of the same underlying phenomenon. In particular, it is unknown whether PINNs introduce new sources of uncertainty that are absent in standard neural networks.

This work investigates the uncertainty landscape of PINNs in comparison with conventional neural networks (NNs). Building on the established decomposition of uncertainty into epistemic (missing knowledge and aleatoric (underlying randomness), we argue that these two categories are insufficient to describe all uncertainty contributors in data-driven engineering models. We therefore propose a systematic taxonomy that traces uncertainty back to distinct stages of the development workflow: data acquisition, preprocessing, model formulation, training, and validation.

The methodology proceeds in two phases. First, an academic benchmark problem is used to train a NN and a PINN on identical data. Both models are evaluated regarding uncertainties and their sources in the development process, while additional diagnostics capture physics-related uncertainties. The comparative analysis reveals which uncertainty sources are mitigated by the physics-informed loss and which persist or emerge.

Second, the insights obtained from the controlled experiment are transferred to the construction of PINN-based surrogate models for a realistic engineering application in the context of a surrogate model for an engine condition monitoring where data driven model are utilized. By explicitly accounting for the identified uncertainty contributors, we demonstrate how to evaluate the model uncertainty and model robustness under operating-point variations.

Overall, the study provides a comprehensive framework for evaluating and quantifying uncertainties in PINNs, thereby enabling more reliable deployment of physics-guided machine-learning surrogates in engineering practice.

**Deep Learning methods for stochastic Galerkin approximations of elliptic random PDEs**

Musco, Fabio; Barth, Andrea 09:30
*University of Stuttgart, Germany*

We consider stochastic Galerkin approximations of linear elliptic partial differential equations. A classical numerical solver for the resulting high-dimensional coupled system of PDEs is replaced by deep learning approaches. In order to achieve this, physics-informed neural networks (PINNs), which typically operate on the strong residual of the PDE and can therefore be applied in a wide range of settings, are considered. As a second approach, the Deep Ritz method, which is a neural network that minimizes the Ritz energy functional to find the weak solution, is employed. While the second approach only works in special cases, it overcomes the necessity of testing in variational problems while maintaining mathematical rigor and ensuring the existence of a unique solution. Furthermore, the residual is of a lower differentiation order, reducing the training cost considerably.

**Neural-Network-Driven Sequential Quasi Monte Carlo Sampling for Bayesian Inference with Complex Posteriors**

Panagiotopoulos, Andreas (1); Mudassar, Javed (2); Repke, Jens-Uwe (2); Brösigke, Georg (2); Matera, Sebastian (1) 09:50
*1: Fritz Haber Institut der MPG, Germany*
*2: Technische Universität Berlin*

Bayesian inference has become increasingly prominent due to its systematic treatment of uncertainty and its advantages over classical parameter estimation. Yet these benefits come with the challenge of sampling high-dimensional parameter spaces, a task that becomes computationally intensive for nonlinear and highly sensitive forward models. The difficulty is amplified when uninformative priors meet accurate data, producing sharply localized and intricate posterior distributions that pose significant obstacles for standard sampling algorithms.

To address this, we introduce a sequential importance sampling framework that employs neural-network normalizing flows in combination with Quasi–Monte Carlo (QMC) techniques. The method proceeds by first learning a coarse approximation of the posterior through a simple initial proposal distribution, forming the first layer of the normalizing flow. QMC sampling through this learned transformation then generates structured samples for refining subsequent flow layers. Because early stages of the procedure encounter distributions too concentrated to sample effectively, we incorporate a tempering strategy that stabilizes the learning and sampling process.

We illustrate the performance and mathematical behavior of the method on a challenging inverse problem arising from chemical kinetics, where the resulting posteriors are very complex. The framework highlights how flow-based transformations and QMC structure can be combined to tackle complex Bayesian inference problems in high dimensions.

## S15.07: Uncertainty Quantification for Dynamical Systems

Date: March 19, 2026 14:00–16:00
Room: KII, M17.21

**Uncertainty Quantification for Bifurcating Dynamical Systems**

Lux-Gottschalk, Kerstin (1); Ernst, Oliver (2); Sprungk, Björn (3) 14:00
*1: Eindhoven University of Technology, Netherlands, The*
*2: TU Chemnitz*
*3: TU Freiberg*

Many real-world systems can be modeled in terms of systems of differential equations. Oftentimes, the dynamics are inherently nonlinear, which means that sudden, large and irreversible changes can occur when an external forcing parameter is varied. Here, we analyze some of these prototypical

bifurcation dynamics in the realm of uncertainty [1]. In this talk, we will consider parameter uncertainty. This arises naturally when model parameters are not known exactly or need to be estimated from data.

We will kickoff the talk with a short introduction of the double fold bifurcation and illustration of how parameter uncertainty can crucially alter the equilibria of a system and their stability properties. Since there often is ambiguity about the exact distribution of uncertain model parameters, we extend classical bifurcation analysis by an uncertainty quantification for different model input parameter distributions. For a given input distribution of an uncertain model parameter, we obtain a probabilistic family of corresponding equilibria along so-called bifurcation curves instead of just a single curve. We transfer results from [2] to bifurcation theory. We address how sensitive these bifurcation curves react to changes in the model input distribution. We propose relevant quantities of interest (QoIs) and prove their Lipschitz- or Hölder continuous dependence on the model input parameter. We consider relevant risk measures and derive bounds for both the QoIs and corresponding risk measures in terms of distances of model input parameter distributions.

This talk covers joint work with Oliver Ernst (TU Chemnitz) and Björn Sprungk (TU Freiberg).

[1] K. Lux, P. Ashwin, R. Wood, and C. Kuehn. Assessing the impact of parametric uncertainty on tipping points of the Atlantic meridional overturning circulation. Environmental Research Letters, 17(7):075002, 2022.

[2] O. G. Ernst, A. Pichler, and B. Sprungk. Wasserstein Sensitivity of Risk and Uncertainty Propagation, 10(3), 2022.

**A modeling perspective on uncertainties in dynamical systems**

Tüting, Katja; Langemann, Dirk
*Technische Universität Braunschweig, Germany*

14:40

We describe a modeling perspective on uncertainty quantification (UQ) in deterministic dynamical systems.

For an uncertain initial state and additional system uncertainties, the time-dependent states are a stochastic process following a stochastic differential equation. Under some regularity conditions, the random variables are described by their probability densities and the time evolution of the density is given by the Fokker-Planck equation.

The Fokker-Planck equation is the best and at least theoretically available analytic description of the uncertainties in a dynamical system. Although solving the Fokker-Planck equation is not feasible in most applications, it can serve as a reference for practical UQ models. We derive a family of UQ models of different fidelity including the classical update schemes of the mean value and the covariance matrix. For these classical update schemes, we discuss indicators for the approximation quality and for step-size control.

The Fokker-Planck equation is our reference model or ground truth and this reference allows the evaluation of the other models in our model family. We discuss an abstract modeling perspective on this family of models and compare it to established theories like the numerics of ODEs.

**Weak error estimates of LOD for multiscale SPDEs**

Hermann, Martin (1); Lang, Annika (2); Målqvist, Axel (2)
*1: Universität Augsburg, Germany*
*2: Chalmers University of Technology*

15:00

The Localized Orthogonal Decomposition (LOD) method is used in numerical homogenization to incorporate fine-scale structure into the solution of a partial differential equation that strongly oscillates in space. When combined with additive noise in time, the interaction of regularities results in a complex setting for the analyis of the corresponding convergence behaviour. We present corresponding theoretical results and numerical verifications.

**Towards one-shot multifidelity methods for compute intensive models**

Kuhn, Allan; Dölz, Jürgen
*University of Bonn, Germany*

15:20

In uncertainty quantification, multifidelity methods use model hierarchies to reduce the computational burden of Monte Carlo simulations. However, for compute intensive models, these computational burdens can still be computationally prohibitive. Using examples from Molecular Dynamics, we examine how established techniques, including multifidelity Monte Carlo, can deliver substantial computational speed-ups, but also that they are still subject to computational constraints. Based on these observations, we outline how exploiting regularity and small-noise structure may be explored for a perturbation based multifidelity expansion, which relies on only one high-fidelity model evaluation. Numerical examples will be provided to illustrate the results.

## S16: Optimization

Organizer(s): De Marchi, Alberto *(University of the Bundeswehr Munich)*
Hansknecht, Christoph *(TU Clausthal)*

## S16.01: Nonlinear Optimization Algorithms

Date: March 18, 2026 08:30–09:30
Room: KII, M17.81
Chair(s): Hansknecht, Christoph
De Marchi, Alberto

### Numerical Approaches to Regularized Nonlinear Programming

De Marchi, Alberto 08:30
*University of the Bundeswehr Munich, Germany*

How can we solve minimization problems with structured objective function (sum of a smooth and a prox-friendly term) and smooth constraints? Penalty, augmented Lagrangian and barrier schemes have been proposed to tackle this problem class, exploiting off-the-shelf proximal-gradient methods as subsolvers. In this talk we take on a different approach, one that was hidden in plain sight. It will be illustrated how to develop methods for this broad problem class, with appropriate convergence guarantees in the fully nonconvex setting, relying on mature nonlinear programming technology.

### Input-to-state stability of Newton-type nonlinear optimization algorithms

Cunis, Torbjørn (1,2) 08:50
*1: University of Stuttgart, Germany*
*2: University of Michigan, USA*

Modern cyber-physical systems increasingly employ advanced nonlinear optimization algorithms for guidance and control. Applications include optimal path planning, collision avoidance, model predictive control, extremum seeking, and online learning for data-driven adaption. This has motivated the study of stability and robustness of nonlinear optimization algorithms in the context of dynamics systems and control theory.

Previous results have shown that strong (metric) regularity of the Karush–Kuhn–Tucker (KKT) system of necessary conditions for optimality are *sufficient* for local input-to-state stability (ISS) of generalized Newton methods to small disturbances. Newton-type optimization algorithms include sequential quadratic programming, its variants sequential linear and convex programing, and augmented Lagrangian methods. Strong regularity is a concept from variational analysis that characterizes the Lipschitz stability of primal-dual solutions under perturbations. However, strong regularity of the KKT conditions implies local uniqueness of the primal-dual solution and is often a very strong assumption.

In this work, we give a *necessary* characterization of strong regularity of the KKT conditions in the form of an incremental ISS property for Newton-type algorithms. Specifically, we show that generalized Newton methods are locally incrementally ISS if and only if the KKT conditions have the strong regularity property. Moreover, we discuss the ISS property of Newton-type algorithms for optimization, possibly with globalization strategies, under the mild additional assumption of local monotonicity. Our results indicate a connection of ISS to the recently proposed concept of *variational convexity* as necessary condition for optimality.

### Unconstrained optimization of polyconvex functionals

Fehling, Marc (1); Tůma, Karel (1); Schwarzacher, Sebastian (1,2) 09:10
*1: Charles University, Czech Republic (Czechia)*
*2: Uppsala University, Sweden*

Minimizers of polyconvex functionals play an essential role in nonlinear elasticity, yet showing their uniqueness remains an open problem. In this work, we investigate this problem through numerical optimization.

Our approach formulates the large deformation problem as an unconstrained optimization over continuous piecewise polynomials. Given boundary displacements and an energy functional, we compute the displacement field minimizing the total energy of the body.
Our prototype implementation leverages the open-source libraries ROL for numerical optimization, deal.II for finite element discretization, and Sacado for automatic differentiation. We present preliminary results for a buckling problem to demonstrate the method's potential, alongside initial attempts to make claims on the uniqueness of minimizers.

## S16.02: Discrete Optimization

Date: March 18, 2026 14:00–16:00
Room: KII, M17.81
Chair(s): Hansknecht, Christoph
De Marchi, Alberto

### A biased Introduction to Discrete Optimization and Machine Learning

Pokutta, Sebastian 14:00
*Zuse Institute Berlin and TU Berlin, Germany*

This talk centers on Frank–Wolfe methods (also known as conditional gradient methods) for constrained optimization, with an emphasis on their role at the interface of discrete optimization and machine learning. These first-order algorithms are particularly well suited for minimizing smooth convex objectives over combinatorial and polyhedral feasible sets, where projection-free updates exploit underlying discrete structure via linear optimization oracles. Originally developed for classical continuous optimization, Frank–Wolfe methods have recently gained renewed attention in machine learning due to their ability to preserve structure, induce sparsity, and scale to high-dimensional problems with complex constraints. I will give a broad overview of the algorithmic principles underlying these methods, discuss their connections to discrete optimization, and highlight recent advances and applications in modern machine learning. Time permitting, I will also outline extensions of Frank–Wolfe techniques to mixed-integer convex optimization, further strengthening the link between continuous and discrete optimization paradigms.

### Two-Echelon Multi-Compartment Vehicle Routing Problem With Facility Location

Byatur, Büşra (1); Özceylan, Eren (1); Karaoğlan, İsmail (2) 14:40
*1: Industrial Engineering Department, Gaziantep University, Gaziantep, 27010, Turkey*
*2: Department of Industrial Engineering, Konya Technical University, Konya, Turkey*

A fully integrated solar energy installation system consists of basic components such as monocrystalline or polycrystalline photovoltaic panels, high-efficiency microinverters, and aluminum mounting profiles. While the average economic and technical lifespan of photovoltaic panels is approximately 25 years, the operational lifespan of inverters is limited to around 15 years. Upon reaching the end of these periods, panels and inverters that have completed their useful life must be collected from installation sites and directed into appropriate recycling or disposal processes.

Photovoltaic panels can be disassembled into distinct material categories such as aluminum, glass, and electronic waste through preliminary sorting procedures conducted either on-site or at transfer points. In contrast, end-of-life inverters must be transported intact, with their structural integrity preserved, in order to be incorporated into recycling or potential reuse processes. This requirement necessitates the management of heterogeneous waste streams with differing transportation and handling specifications within a unified logistics network.

The problem addressed in this study is characterized by a two-echelon reverse logistics network structure that involves the collection of solar photovoltaic system waste subjected to on-site pre-sorting, and its transportation to designated separation centers and final recycling facilities. Within this network structure, a Multi-Compartment Vehicle Routing Problem (MCVRP) is considered, in which vehicles equipped with separate compartments for different waste types are employed. In addition, the locations of the separation centers are included among the decision variables, and the problem

integrally incorporates vehicle routing, intermediate node location, and two-echelon network design decisions within a single framework.

Accordingly, a comprehensive mathematical model has been developed to address the problem. Experimental analyses have been conducted across test scenarios of varying scales to validate the computational performance and effectiveness of the proposed model.

**Residual Simplex method for solving large-scale linear programming problems**

Vanroose, Wim; Van Thienen, sebastian; Symoens, Bas 15:00
*U Antwerpen, Belgium*

We present the residual simplex method, a framework for solving large-scale linear programming (LP) problems by decomposing them into a sequence of smaller, more tractable subproblems. Rather than working directly in the full space of variables, the method operates in subspaces defined by the residuals of the linear constraints, leading to a projected LP at each iteration.
Each projected problem can be solved efficiently using standard tools such as the dual simplex method or gradient-based ascent schemes. Viewed from the dual perspective, the algorithm performs an ascent along mutually orthogonal directions, providing a clear geometric interpretation of the method. This structure makes the residual simplex approach particularly effective for highly degenerate LPs, where many basic variables lie on their lower or upper bounds—a setting in which classical simplex-type methods often struggle.
In this talk, we review the definition of the residual simplex method and discuss its main theoretical properties. We show how the projection framework naturally connects the method to Krylov subspace techniques, thereby linking linear programming with ideas from numerical linear algebra and iterative methods. These connections offer additional insight into both the behavior and the computational efficiency of the algorithm.
We also address practical aspects of the method, including convergence properties and the role of accuracy in solving the intermediate auxiliary subproblems. In particular, we discuss how the tolerances used in these subproblems influence overall performance and robustness.
The methodology is illustrated using large-scale scheduling problems arising in the airline industry, where LPs with millions of variables and constraints are common and degeneracy is pervasive. These examples demonstrate how the residual simplex method can exploit problem structure to achieve significant computational gains.

**An Online Budgeted-Robust Variant of CTOP: Tight Competitive Guarantees and Real-Time Heuristics**

Sayin, Mesut 15:20
*Ozyegin University, Turkey (Türkiye)*

We study an online, budgeted-robust extension of the Capacitated Team Orienteering Problem (CTOP), termed OR-CTOP, in which routing decisions must be made while key problem data are uncertain. The uncertainty simultaneously affects node rewards (prizes), customer loads (demands/weights), service durations, and arc travel times. We model these perturbations via a budget uncertainty set, and consider an online information structure where uncertain coefficients are revealed sequentially over time to the decision maker, thereby coupling robust decision-making with online feasibility and performance considerations.

To assess algorithmic quality in this setting, we adopt a competitive analysis framework and measure performance via the competitive ratio (CR). Recognizing that worst-case CR can be excessively conservative, we introduce a setup-based competitive benchmark that evaluates an online policy relative to an arbitrary decision-maker–specified reference instance. Under this refined notion, we derive a tight lower bound on the setup-based CR attainable by any online algorithm for OR-CTOP, which quantifies, under adversarial realizations, the maximal value of perfect foresight compared with online decision-making.

Building on this characterization, we develop two formulation-driven online methods: (i) a static robust policy and (ii) an adaptive robust policy that updates decisions as uncertainty is disclosed. For

each method, we prove setup-based CR guarantees that match the tight lower bound, establishing worst-case optimality within the proposed benchmarking regime. We further complement worst-case theory with an average-case analysis, showing that the adaptive method dominates the static one in expected performance and achieves a strictly improved average-case CR.

To support real-time operational deployment, we design robust evolutionary heuristics that rapidly approximate the solutions implied by both formulation-based methods at decision time. We validate the proposed approaches on instances derived from real urban transportation networks in regions impacted by the 2023 Türkiye earthquake. Extensive computational experiments demonstrate that the heuristics closely track their corresponding mathematical formulations and that the adaptive algorithm consistently outperforms the static algorithm in terms of average-case competitive performance.

**A Framework for the Solution of Tree-Coupled Saddle-Point Systems**

Hansknecht, Christoph (1); Heinzelreiter, Bernhard (2); Pearson, John (2); Potschka, Andreas (1) 15:40
*1: TU Clausthal, Germany*
*2: The University of Edinburgh*

We consider the solution of saddle-point systems with a tree-based block structure, introducing a parallelizable direct method for their solution. As our key contribution, we then propose several structure-exploiting preconditioners to be used during applications of the GMRES algorithm and analyze their properties. We adapt several concepts originating in the field of multigrid methods, obtaining a variety of problem-adapted multi-level methods. We analyze the complexity of all algorithms, and derive a number of results on eigenvalues of the preconditioned system and convergence of iterative methods. We validate our theoretical findings through a range of numerical experiments.

## S16.03: Modeling and Multi-Criteria Optimization

Date: March 18, 2026 16:30–18:30
Room: KII, M17.81
Chair(s): Hansknecht, Christoph
De Marchi, Alberto

**A compromise programming approach for assessing enterprise competitiveness based on a three-level hierarchy of criteria**

Kao, Chiang 16:30
*National Cheng Kung University, Taiwan*

In multicriteria decision making (MCDM), a set of alternatives are compared based on a number of criteria. The alternative with the best aggregate performance of the criteria is selected to undertake. For complicated problems with many criteria to consider, the criteria are categorized into groups at different levels for analysis. For example, the competitiveness of a company can be assessed from the aspects of past performance and future potential at the first level. Under each aspect there are several subjects to consider. The aspect of past performance, for instance, can be assessed from the subjects of productivity and profitability at the second level. Each subject is then assessed from a number of criteria at the third level. For example, the productivity subject can be assessed from the criteria of operating productivity, labor productivity, and assets productivity. In this case, one has a three-level hierarchy MCDM problem. This paper discusses the assessment of the alternatives with a three-level hierarchy of criteria where suitable weights for the criteria at different levels are sought. A compromise programming model is developed to find the weights. The problem is solved in two stages. The first stage calculates the most favorable weights that produce the highest score, or ideal score, for each alternative. The second stage determines a set of common weights that is able to produce the final scores that are closest to the ideal scores for all alternatives in an aggregate sense. Due to the three-level structure, the models in the two stages are nonlinear. By applying a variable substitution technique and a golden section search technique, the problem of the first stage becomes solving a sequence of linear programs and that of the second stage becomes solving a sequence of quadratic programs. Each alternative requires solving no more than fifteen linear programs to obtain

the most favorable weights with a precision of four decimal digits in the first stage. Similarly, no more than fifteen quadratic programs are required to solve to obtain the common weights for all alternatives in the second stage. The model is applied to measure the enterprise competitiveness of 1,801 listed companies in Taiwan. Based on the competitiveness indexes, the competitiveness of the 1,801 companies are ranked. As competitions among companies for limited markets become increasingly fierce, companies must be more competitive to survive and prosper. From the aspect and subject scores, the strengths and weaknesses of a company are identified. Maintaining the strengths and improving the weaknesses enhances the competitiveness of the company.

**On extended real-valued variational inequalities - stability and penalization**

Gwinner, Joachim 16:50
*Universität der Bundeswehr München, Germany*

In this talk we address a class of constrained extended real-valued variational inequalities and present a general stability theorem. From this theorem we derive convergence results for a penalization procedure. As an application we treat a nonlinear boundary value problem that models unilateral contact problems of continuum mechanics with non-monotone friction.

Some references:

J. Gwinner, On the penalty method for constrained variational inequalities, Optimization,theory and algorithms, Lect. Notes Pure Appl. Math. 86, 197-211 (1983).

J. Gwinner, From the Fan-KKM principle to extended real-valued equilibria and to variational-hemivariational inequalities with application to nonmonotone contact problems, Fixed Point Theory Algorithms Sci. Eng., 2022, 28 pp.

**A framework for the optimal modeling of rubber-like materials**

Houari, Fadoua; Caylak, Ismail; Ostwald, Richard 17:10
*Chair of Structural and Materials Mechanics (SWM), University of Paderborn*

In the modeling of rubber-like materials, parameter identification is typically performed using a least squares optimization that fits constitutive models to experimental data. Although this approach often provides excellent agreement for a particular strain mode (verification), the resulting parameters may lack robustness under different loading scenarios and can exhibit instability. Two primary sources of this behavior are identified: model deficiency, where an excessive number of parameters in the constitutive model introduces near-linear dependencies and weak identifiability [1], and data deficiency, where the available experiments do not sufficiently activate all deformation mechanisms represented by the model. Unlike the classical approches of parameter identification (cf. e.g., [2]), we propose an integrated framework for modeling rubber-like materials and parameter identification that systematically combines verification, stability, and validation. Stability is quantified using optimal experimental design criteria $\Phi_I$. The framework is applied to Treloar's classic rubber data (Trans. Faraday Soc. 40:59–70, 1944) [3] and to twelve hyperelastic models. Among these, the Carroll model demonstrates the best overall performance, providing accurate fits, stable parameter set, and strong predictive capability across multiple loading modes.

References:

1. I. Caylak, E. Penner, A. Dridger, and R. Mahnken. Stochastic hyperelastic modeling considering dependency of material parameters. Computational Mechanics, 62(4):859–876, 2018.

2. A. Schowtjak, R. Schulte, T. Clausmeyer, R. Ostwald, A. E. Tekkaya, and A. Menzel. Adapt — a diversely applicable parameter identification tool: Overview and full-field application examples. International Journal of Mechanical Sciences, 213:106840, 2022.

3. L. R. G. Treloar. Stress-strain data for vulcanised rubber under various types of deformation. Transactions of the Faraday Society, 40:59–70, 1944.

**Simultaneous Optimization of Design Layout and Material Properties in Reinforced Concrete Structures**

Masarczyk, Daniela (1); Tran, Minh Tuan (2); Kuhl, Detlef (1) 17:30
*1: University of Kassel, Germany*
*2: Vietnamese German University, Vietnam*

Concrete, the most popular building material in civil engineering, is characterized by a pronounced anisotropy in tensile and compressive strength, with its compressive strength exceeding the tensile strength by approximately a factor of ten [1]. This limitation is mitigated through the introduction of steel reinforcement into fresh concrete, resulting in an anisotropic composite material. The aim of this study is to develop a topology optimization model that accounts for the material properties of reinforced concrete and thus simultaneously optimizes both the structural layout and the steel reinforcement layout.

Topology optimization can significantly facilitate the early design stages of resource efficient civil engineering structures and enable improved performance with respect to selected mechanical criteria. The typical design task consists of a material distribution problem in a FE discretized design space. Load transfer primarily by normal forces, a key criterion of mechanical efficiency, is ensured by minimization of the elastic strain energy [2].

This work investigates the simultaneous optimization of structural design and local material properties using a SIMP-based topology optimization framework. Reinforced concrete is represented using a smeared, macroscopic approach based on the theory of mixtures [3] and the concept of volume fractions [4]. The composite material is modeled as bundles of unidirectional steel fibers embedded in a concrete matrix, which enhance tensile strength and material stiffness along their orientation. Simultaneous optimization of design layout and material properties is achieved by extending the design variable vector describing the material distribution in the design space, to include the volume fraction and the orientation of the steel reinforcement. A penalization scheme is introduced to distribute the reinforcement to areas primarily subjected to tensile loading. The presented approaches are thoroughly tested, the interaction between the different design variables is analyzed, and the method is evaluated.

[1] A. E. Jacintho, et al., Modulus and strength of concretes with alternative materials, Materials 13, 4378 (2020).
[2] D. Masarczyk, and D. Kuhl, Topology optimization considering self-weight, Proc. Appl. Math. 23, e202300258 (2023).
[3] R. M. Bowen, Theory of Mixtures, A. C. Eringen, Continuum Physics 3, 1 – 127 (1976).
[4] R. de Boer, and W. Ehlers, On the problem of fluid- and gas-filled elasto-plastic solids, Int. J. Solids Structures 22 (11), 1231 – 1242 (1986).

**Knowledge Infused Bayesian Optimization of Hyperparameters for Inverse Problems**

Hornischer, Niklas (1); Blessing, Lea (1); Huber, Felix (1); Barth, Andrea (1,2); Göddeke, Dominik (1,2) 17:50
*1: University of Stuttgart, Germany*
*2: Stuttgart Center for Simulation Science (SC SimTech), Germany*

Solving optimization, uncertainty quantification, and inverse problems generally entails repeated evaluations of high-fidelity forward models for numerous parameter configurations. Consequently, the computational load imposes a hard to overcome practical barrier limiting the applicability of established methods. This often prevents parameter studies of these types from being conducted with sufficient resolution or accuracy.

While many approaches to reduce the computational burden of numerical methods, like surrogate modeling and machine learning, exist, they mainly provide approximations to the considered forward models. Not only by introducing additional errors, but also since their construction typically involves a high number of samples of the involved forward models, the use cases of these approaches are restricted.

A critical yet largely unsystematically treated aspect in this context is the selection of hyperparameters that directly govern the behavior of the involved numerical approaches. In contrast to the parameters under investigation in the parameter study itself, hyperparameters directly influence the numerical performance in terms of accuracy, convergence and runtime. In practice, however, they are usually chosen manually and heuristically, which can lead to suboptimal settings.

We present a general framework for the systematic constrained optimization of hyperparameters within parameter studies. At the core we incorporate available a priori knowledge about numerical methods into a Bayesian Optimization strategy. By guiding the search process with this infused knowledge, we aim at balancing adaptability and robustness while incurring only a modest computational overhead.
Samples generated within this optimization loop are not only relevant for understanding the behavior of the simulation but can also be reused in the surrounding parameter study, further reducing the overall computational overhead of our approach.

With hyperparameters influencing the performance and accuracy of almost any numerical method, we focus on PDE-based applications where the computational cost of even a single model evaluation can be substantial. We demonstrate the applicability of the approach by focusing on inverse problems which typically require a high number of samples to obtain usable and precise results.

## S16.04: Non-Smoothness and Complementarity Constraints

Date: March 19, 2026 08:30–10:30
Room: KII, M17.81
Chair(s): De Marchi, Alberto
Hansknecht, Christoph

### On optimality conditions for nonsmooth functions

Walther, Andrea 08:30
*Humboldt-Universität zu Berlin, Germany*

Numerous optimization tasks exhibit a nonsmooth behavior. In contrast to the classical smooth case, where optimality conditions are well studied and understood, criteria to determine whether a given point is optimal or even just stationary are still the subject of ongoing research for nonsmooth functions to be minimized.
In this talk, I will first introduce already established optimality conditions based on generalized derivative concepts for unconstrained nonsmooth problems. Subsequently, we will discuss new optimality conditions for a large class of piecewise smooth functions using so-called kink qualifications. Here, the computational complexity to verify the new criteria is also covered. Finally, I will present important properties of the kink qualification LIKQ.

### An adaptive semismooth Newton method with global convergence rates

Alphonse, Amal; Dvurechensky, Pavel; Papadopoulos, Ioannis P. A.; Sirotenko, Clemens 09:10
*WIAS, Germany*

I will discuss a semismooth Newton-type method with a simple, parameter-free globalisation strategy that guarantees convergence from arbitrary starting points to stationary points, and under a PL condition, to a global minimum, in Hilbert spaces. The method employs an adaptive Levenberg–Marquardt regularisation for the Newton steps and does not require knowledge of problem-specific constants. I will show that it achieves certain global rates under various settings, and also local superlinear convergence under semismoothness and Dennis–Moré or partial smoothness conditions. Some examples selected from imaging, contact mechanics, and machine learning will conclude the talk.

**A Globally Convergent Method for Computing B-stationary Points of Mathematical Programs with Equilibrium Constraints**

Nurkanovic, Armin (1); Leyffer, Sven (2)
*1: University of Freiburg, Germany*
*2: Argonne National Laboratory, USA*

09:30

This talk presents a computationally efficient method that globally converges to B-stationary points of mathematical programs with equilibrium constraints (MPECs) in a finite number of iterations. B-stationarity is a necessary condition for optimality, indicating that no feasible first-order direction can improve the objective. Given a feasible point of an MPEC, B-stationarity can be certified by solving a linear program with equilibrium constraints (LPEC) constructed at that point.
The proposed method solves a sequence LPECs, which either certify B-stationarity or provide an active-set estimate for the complementarity constraints, as well as a sequence of nonlinear programs (NLPs), referred to as branch NLPs (BNLPs), obtained by fixing the active set in the MPEC.
A BNLP is more regular than the original MPEC, easier to solve, and, when the active set is correctly identified its solution coincides with that of the MPEC.
We show that, unless the current iterate is B-stationary, the combinatorial LPECs need not be solved to optimality; for convergence, it suffices to compute a nonzero feasible point, yielding significant computational savings. The method proceeds in two phases: the first identifies a feasible BNLP or a stationary point of a constraint-infeasibility minimization problem, and the second solves a sequence of BNLPs until a B-stationary point of the MPEC is found. We establish finite convergence under the MPEC-MFCQ. Numerical experiments and an open-source implementation demonstrate that the proposed method is more robust and faster than relaxation-based and mixed-integer NLP approaches, even on medium- to large-scale instances.

**High-Performance Solvers for Large-Scale Mathematical Programs with Complementarity Constraints**

Pozharskiy, Anton Edvinovich (1); Nurkanović, Armin (1); Pacaud, François (2); Diehl, Moritz (1)
*1: Universität Freiburg, Freiburg im Breisgau, Germany*
*2: Mines Paris-PSL, Paris, France*

09:50

We present a Julia package, built on top of MadNLP, implementing a suite of algorithms for Mathematical Programs with Complementarity Constraints (MPCCs). MPCCs have recently gained renewed attention in engineering optimization, as complementarity provides a powerful modeling tool for non-smooth functions. These problems are inherently challenging since their nonlinear programming reformulations violate classical regularity conditions at all feasible points, complicating both theoretical analysis and numerical treatment. Consequently, specialized algorithms are required to handle this degeneracy. We implement a toolbox of such methods, including relaxation and penalty approaches, as well as a crossover to recently proposed active-set methods. Our solver is based on nonlinear interior-point algorithms, where in addition the relaxation or penalty parameter is coupled with the barrier parameter, yielding substantial speedups compared to standard implementations. We discuss implementation details such as new nonmonotone strategies for joint barrier and relaxation parameter updates. Further, several techniques for handling the ill-conditioning of the KKT matrix near solutions are proposed. Finally, we validate our implementation and show significant computational speedups both on the classical MacMPEC benchmark, as well as on a new benchmark suite made up of large scale problems coming from the optimal control of nonsmooth systems, security constrained optimal power flow, as well as other real-world MPCCs.

**Contact-Implicit Inverse Dynamics**

Ménager, Etienne (1); Fabre, Pierre (1); Bambade, Antoine (2); Jallet, Wilson (1); De Marchi, Alberto (3); Carpentier, Justin (1) 10:10

*1: INRIA, France*
*2: EDF Lab*
*3: University of the Bundeswehr Munich*

Task-space inverse dynamics, also known as operational space control, is a popular control paradigm for controlling robots in real-time. It enables the control or stabilization of robot dynamics around reference trajectories while accounting for under-actuation, actuator limits, and contact interactions. Over the past few decades, this versatile control paradigm has been successfully deployed in numerous robotics settings, ranging from quadrupeds and humanoid robots to deformable robots, in scenarios involving rich physical contact interactions between a robot and its environment. In practice, contact-aware inverse dynamics controllers assume that contact sequences are known in advance, typically provided by a higher-level contact planner, which inherently limits their ability to select among breaking, sliding, or sticking contacts automatically.

In this work, we extend the control formalism of task-space inverse dynamics, which is classically formulated as a quadratic program, to a more general quadratic program with complementarity constraints (QPCC). This formulation fully accounts for actuator limits and frictional contacts, modeled as nonlinear complementary constraints. To solve these QPCC problems, we draw inspiration from the alternating direction method of multipliers to devise an iterative optimization approach that alternates between minimizing a smooth convex function that accounts for task objectives and system dynamics, and projecting over convex and non-convex sets that capture actuator and complementary frictional contact constraints. By notably handling complementary frictional contact constraints through projection, our approach enables us to implicitly and automatically reason about the optimal contact modes that fulfill the task objectives and constraints.

We have implemented our QPCC solver in C++ for efficiency, and demonstrate its usability and versatility on rigid and soft robots across various control scenarios, ranging from the control of actuated box sliding on the grounds, to control balance of legged robots that automatically break and create contacts (e.g., jumping tasks, balancing tasks) or control of deformable robots interacting with their environment.

## S16.05: PDE-Constrained Optimization and Model Reduction

Date: March 20, 2026 08:30–10:30
Room: KII, M17.81
Chair(s): De Marchi, Alberto
Hansknecht, Christoph

**Topology Optimization for Grayscale Masked Stereolithography**

Rutsch, Felix; Weeger, Oliver 08:30

*TU Darmstadt, Germany*

In a grayscale masked stereolithography apparatus (gMSLA), a liquid polymer resin is selectively exposed to UV light in a layer-by-layer fashion to create three-dimensional structures. The light exposure of each point can be adjusted accurately by varying the local grayscale value displayed on a projection LCD mask situated below the resin tank. This determines where the material is cured or remains liquid within each layer. In addition, the dose of light exposure determines the material properties, such that the local stiffness of the material increases with higher exposure. At this point, light propagation effects play a decisive role, leading to overcuring, i.e., a mismatch between the original CAD geometries and the print results. A simulation of the printing process including these effects enables an accurate prediction of the geometry and properties of the printed object and can be used for optimization.

Topology optimization (TO) of structures is a research field of growing interest. TO can be used to maximize the stiffness of a structure with fixed amount of material, to obtain optimal designs for

compliant mechanisms, or to generate microstructures. The complex optimized designs are often challenging to manufacture, where additive manufacturing processes can display their advantages. At this point, it can be important to include a simulation of the printing process in the TO, in order to take into account the characteristics of the print process and obtain designs that can directly be additively manufactured with high accuracy.

The authors investigate how the aforementioned gMSLA process simulation can be integrated into the TO. The grayscale input masks are used as design variables, such that the optimization result can directly be printed. The dependency of the material properties on the exposure dose opens up the possibility for TO of functionally graded material designs.

**Topology, orientation and fiber path optimization for layered anisotropic materials**

Jantos, Dustin Roman; Junker, Philipp 08:50
*Leibniz University Hannover (LUH), Germany, Institue of Continuum Mechanics (IKM)*

Topology optimization and additive manufacturing complement each other: the freedom in design optimization allows for the creation of complex, highly efficient structures that are often feasible only through additive manufacturing. However, most structural optimization methods assume isotropic material properties, which contradict the inherent anisotropy of structures produced via additive manufacturing. Therefore, a comprehensive optimization should consider not only the topology but also the local material properties. Additionally, many additive manufacturing processes require support structures to construct overhangs.

The literature contains approaches for optimizing fiber angles, both discrete and continuous, even in three-dimensional problems, typically allowing free material orientation in three-dimensional space. Although such designs could potentially be fabricated using five-axis additive manufacturing, most additive manufacturing processes today limit the fiber orientation or toolpath to remain parallel to a specific plane (three-axis machines) – often referred to as the printing layers, typically denoted by the z-axis normal of the machine. Additionally, specific constraints on the curvature of fibers or tool paths within the layer plane may apply. Depending on the specific manufacturing process, these restrictions can significantly impact not only the material properties but also the optimal topology.

We present a optimization approach for the topology of layered anisotropic materials, which includes optimizing the global print plane, local fiber or tool paths, and additionally restricting the maximum fiber curvature within the layers. The potential to restrict and reduce overhangs is also considered. This approach is grounded in a thermodynamic optimization based on the stationary condition of a variational principle known in thermodynamically consistent material modeling. Transient partial differential equations for the design variables are derived, whose solutions over pseudo-time serve as an update scheme to drive the design variables towards the optimum.

**Optimal Control of Heating Networks under Demand Uncertainty**

Heidrich, Johanna 09:10
*Fraunhofer ITWM, Germany*

In the context of the energy system transition, the operation of district heating networks poses significant challenges that require advanced methods in network simulation and optimization. In particular, the increasing integration of decentralized feed-in substantially complicates the hydraulic behavior of the system. Efficient operation and well-founded expansion decisions therefore rely on an accurate representation of energy transport, governed by a coupled thermo-hydraulic PDE system.

The associated PDE-constrained optimization problems depend crucially on heat demand, entering the model as a boundary condition determined by consumer behavior. Hence, predictive optimization requires the availability of a realistic and mathematically consistent demand forecast model.

To capture systematic demand patterns, we employ gradient boosting methods to obtain temperature-dependent, time-resolved point as well as quantile forecasts. While the deterministic component is accurately described, the residual process can be modeled stochastically based on a

Cox–Ingersoll–Ross–type diffusion with time-varying coefficients, where the diffusion coefficient is linked to the forecast and exogenous variables.

The resulting hybrid model combines data-driven prediction with stochastic process theory and provides a probabilistic representation of demand uncertainty. The optimal control problem is formulated so as to minimize operational costs while ensuring feasibility under stochastic demand uncertainty. To this end, we compare three approaches to incorporate uncertain boundary conditions into the optimization framework: Monte Carlo–based stochastic programming, worst-case robust optimization, and chance-constrained formulations.

**Consistent Variational Shape Gradients Across Finite Elements and Isogeometric Analysis**

Liedmann, Jan 09:30
*University of Stuttgart, Germany*

This work presents a unified framework for variational design sensitivity analysis in both finite element analysis (FEA) and isogeometric analysis (IGA), with the aim of providing a consistent and implementation-friendly route to shape derivatives across different discretization techniques. The formulation is based on a modified kinematic viewpoint that rigorously decouples geometry and physics. This separation enables a clean and systematic derivation of continuum-level shape gradients directly from the underlying weak form, avoiding model-specific manipulations and yielding exact sensitivities at continuum level.

Consistent discretization of these shape gradients using smooth spline spaces naturally leverages the geometric exactness and higher continuity of IGA, while remaining compatible with standard FEA workflows through an equivalent variational structure. The resulting discrete sensitivities inherit the regularity of the chosen approximation spaces and can be evaluated in a stable and reliable manner. By casting the sensitivity problem variationally, the method provides a rigorous basis for numerical implementation, reduces the risk of inconsistencies due to non-systematic discretization choices, and allows the required sensitivity quantities to be computed with only minor additional computational effort beyond the forward analysis.

The accuracy and robustness of the proposed sensitivities are assessed through systematic comparison with finite-difference approximations. In addition, selected shape-optimization examples demonstrate that the framework delivers reliable gradients in practice and supports efficient optimization workflows, even when using smooth geometry parametrizations and higher-order discretizations. These studies highlight that the approach is not only theoretically consistent but also computationally efficient, making it suitable for routine use in gradient-based design optimization.

Beyond the linear-elastic setting, the formulation is extendable to nonlinear material behavior, since the derivation relies on general continuum mechanical principles rather than linear constitutive assumptions. This includes e.g. path-dependent or finite-strain models, provided the corresponding weak forms and consistent linearizations are available. Moreover, the variational structure provides a natural entry point for multi-physics and multi-scale applications. Scale couplings can be incorporated by embedding additional governing equations and their sensitivity contributions within the same unified framework. Overall, the proposed methodology offers a flexible and robust foundation for sensitivity-driven shape design, spanning smooth shape parametrizations, complex material responses, and coupled multi-scale models within a single, consistently discretized variational setting.

**Reactor Shape Optimization for Heterogeneous Catalytic Systems based on Reduced Order CFD**

Qureshi, Muhammad Uzair (1); Paganini, Alberto (2); Brösigke, Georg (1); Repke, Jens-Uwe (1) 09:50
*1: Technische Universität Berlin, Germany*
*2: University of Leicester, UK*

Computational Fluid Dynamics (CFD) analysis of reactive flows over heterogeneous catalysts is a challenging task even for “simple” laminar flows. This involves solving a system of Partial Differential Equations (PDEs) with highly non-linear boundary conditions imposed by the surface chemistry which

leads to stiffness and bad conditioning of the overall equation system requiring extensive computational effort. To address this challenge, we recently developed reduced order models (ROMs) for heterogeneous catalytic systems[1,2]. These ROMs have two advantages: (1) Their pre-processing or offline part is cheaper than other model order reduction methods or machine learning approaches as it does not require solving the high-fidelity simulations and (2) the online part requires only solving non-linear equations (NLEs) rather than a partial differential equation (PDE) system. Since the ROMs enable solving the governing non-linear PDE system with minimal computational effort, it becomes feasible to couple them directly with an optimizer as opposed to full scale CFD. Therefore, one can think of extending these ROMs to applications such as reactor design optimization. In the context of heterogeneous catalysis, this could revolutionize how catalytic reactors are designed especially with the onset of 3D printing techniques.

To this end, we couple the ROMs with the shape optimization toolbox Fireshape[3], which implements a moving-mesh approach to update the computational domain and minimize a target function, which in our case could be the product yield or selectivity. Fireshape has already been used effectively for optimizing geometries where the flow is described by incompressible Navier Stokes.

The complete workflow for optimal reactor design is as follows: The optimizer passes the initial shape to the finite element solver – Firedrake[4] for computation of the non-reactive part of flow comprising the incompressible Navier Stokes equations. The transport properties and velocity fields are computed in this step. Then for the same shape, snapshots (which are PDE systems with piecewise constant Neumann boundary conditions) are generated using Firedrake. The reactive part of the solution is assumed to be a linear combination of these snapshots. The coefficients for each snapshot are then computed via a non-linear algebraic equations' solver. The non-reactive and reactive solutions are combined to estimate the ROM solution. This solution is then passed back to the optimizer which computes the next iterate (shape) based on the gradients computed via automatic differentiation. In this work, we apply this reactor design workflow on different kinetic systems for arbitrary catalytic reactor geometries.

**References:**

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**Don't forget the energy: multi-objective model reduction for port-Hamiltonian systems**

Nicodemus, Jonas (1); Reiter, Sean (2); Unger, Benjamin (1); Gugercin, Serkan (3) 10:10

*1: Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology*

*2: Courant Institute of Mathematical Sciences, New. York University*

*3: Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech*

Model order reduction (MOR) of port-Hamiltonian systems has been extensively studied over the past decades. However, so far little attention has been paid to the energy functional, i.e., the Hamiltonian, which is an intrinsic part of the system. In this paper, we address this issue by formulating the multi-objective MOR problem that simultaneously approximates the input-output mapping and the Hamiltonian. We propose a structure-preserving MOR method based on multi-objective optimization and derive first-order optimality conditions for the resulting problem. Additionally, we derive the Hessian of the cost function, which facilitates two strategies for computing Pareto optimal solutions: a scalarized Newton method and numerical integration along the Pareto front. We illustrate the performance of the proposed method on several numerical examples.

## S17: Applied and numerical linear algebra

Organizer(s): Tabeart, Jemima *(TU Eindhoven)*
Schweitzer, Marcel *(Bergische Universität Wuppertal)*

## S17.01: Matrix equations & matrix functions

Date: March 18, 2026 16:30–18:30
Room: KII, M17.91
Chair(s): Schweitzer, Marcel

### Extrapolation based acceleration of stationary iterations for multi-term matrix equations.

Kürschner, Patrick (1); Benner, Peter (2); Saak, Jens (2); Liu, Xiaobo (2); den Boef, Pascal (3) 16:30
*1: HTWK Leipzig, Germany*
*2: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
*3: Eindhoven University of Technology, Eindhoven, The Netherlands*

We consider the iterative numerical solution of general linear matrix equations
$AX + XB+\Sigma N_k X H_k = -Y$.
For a convergent sequence of vectors, the speed to convergence can be improved by reduced rank extrapolation (RRE) [4]. Here we consider convergent sequences of matrices from iterative methods for matrix equations.
For (low-rank) matrices sequences generated by ADI-type iteration for standard Lyapunov and algebraic Riccati equations, the usage of RRE was recently investigated in [1]. In this presentation, we investigate how these results can be generalized to matrix sequences from (non)stationary iterations [2,3], $X_{j+1}=\Phi_j(X_j)$, for the above multi-term linear matrix equations. We also discuss generalization of the convergence results of [4] for the accelerated sequences in our low-rank algorithms.

References:

1. P. den Boef, P. K¨urschner, X. Liu, J. Maubach, J. Saak, W. Schilders, J. Schulze, and N. van de Wouw. Generalizing reduced rank extrapolation to low-rank matrix sequences. ArXiv:2502.09165, 2025.
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3. S. D. Shank, V. Simoncini, and D. B. Szyld. “Efficient low-rank solution of generalized Lyapunov equations”. Numer. Math. 134 (2015), pp. 327–342.
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### On the Solution of Large-scale Non-autonomous Differential Riccati Equations: a Numerical Study

Mancinelli, Eugenio (1); Palitta, Davide (1); Saak, Jens (2) 17:10
*1: University of Bologna, Italy*
*2: Max Planck Institute for Dynamics of Complex Technical Systems, Germany*

Differential Riccati Equations (DREs) form a class of matrix equations that arise frequently in optimal control and filtering problems, particularly in large-scale systems governed by complex dynamics. The increasing demand from a wide range of applications has stimulated significant research into the design and analysis of efficient numerical algorithms for solving these equations over the years. Most available schemes follow a three-step procedure: (i) the differential operator is discretized in time, e.g., by using Backward Differentiation Formulas (BDFs), resulting in a sequence of nonlinear Algebraic Riccati Equations (AREs); (ii) these nonlinear AREs are then solved; (iii) often via the solution of sequences of linear problems. These phases interact with each other non-trivially leading to some

difficulties in the analysis and performance assessment of the overall numerical procedure, especially in the large-scale setting.

The focus of this study is on large-scale non-autonomous DREs, i.e., equations whose coefficient matrices, and not only the solution, depend on time. In this scenario, only a handful of efficient solvers are available in the literature. In this talk, we present a panel of numerical results aiming at identifying the state-of-the-art solver that best addresses the points (ii) and (iii) above. In particular, we extensively test latest developments regarding the RADI method as inner scheme within the numerical pipeline for the solution of large-scale non-autonomous DREs. Using this method as the inner solver after phase (i) allows the solution of the discretized equations (ii) to be computed directly, bypassing the linearization required by classic Newton-type approaches. This is a joint work with Davide Palitta and Jens Saak.

**Towards a mixed-precision Newton-Kleinman method for the algebraic Riccati equation**

Schulze, Jonas; Saak, Jens
*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*

17:30

Continuous-time algebraic Riccati equations arise in various areas of control theory, for example, linear-quadratic regulator problems and balancing-related model order reduction. For many applications, the coefficient matrices and are large and sparse, while the solution matrix has a low numerical rank. Typical methods to solve such equations are Krylov projection methods, the Newton-Kleinman method, and the RADI method. Meanwhile, mixed-precision techniques have successfully been applied to the Newton-Raphson method, reducing the overall time- and energy-to-solution at virtually no loss of accuracy. We report on our progress of applying mixed-precision techniques to the low-rank Newton-Kleinman method.

**A scaling and recovering algorithm for the matrix $\varphi$-functions**

Liu, Xiaobo (1); Al-Mohy, Awad H. (2)
*1: Max Planck Institute for Dynamics of Complex Technical Systems, Germany*
*2: Department of Mathematics, King Khalid University, Abha, Saudi Arabia*

17:50

A new scaling and recovering algorithm is proposed for simultaneously computing the matrix $\varphi$-functions that arise in exponential integrator methods for the numerical solution of certain first-order systems of ordinary differential equations. The algorithm initially scales the input matrix down by a nonnegative integer power of two, then computes the $[m/m]$ diagonal Padé approximant to $\varphi_p$, where $p$ is the largest index of interest. The remaining $[m+p-j/m]$ Padé approximants to $\varphi_j$, $0 \leq j < p$, are obtained implicitly via a recurrence relation. The effect of scaling is subsequently recovered using the double-argument formula. A rigorous backward error analysis, based on the $[m+p/m]$ Padé approximant to the exponential, enables sharp bounds on the relative backward errors. Numerical experiments demonstrate the superiority of the proposed algorithm over existing alternatives in both accuracy and efficiency.

**Structure preserving computation of the pencil Pad´e approximation**

Diab, Malak; Frommer, Andreas; Kahl, Karsten; Tsolakis, Manuel
*University of Wuppertal, Germany*

18:10

Our work presents structure-preserving computational techniques for the pencil Pad´e approximation and the generalized Cayley transform, arising in the numerical integration of differential-algebraic equations (DAEs) via implicit Runge–Kutta methods such as the implicit mid-point and Gauss–Legendre schemes. We first extend the concept of the diagonal Pad´e approximation and introduce a generalized framework characterizing the s-stage Gauss method. We further examine its structural properties and the role of FOM in approximating the discrete solution. Building on this, we analyze the iterative approximation of the Cayley transform and establish conditions on the search space in Galerkin-type approximations which guarantee that structure-induced properties, such as dissipativity or energy preservation, are inherited by the Galerkin approximations. In particular, we show that FOM-based Krylov subspace methods preserve these properties only when appropriately

augmented or with specific choices of the initial guess. The results provide new insights into the interplay between Krylov subspace methods and energy preservation in the numerical integration of DAEs. We illustrate the convergence and the conservation of the physical properties via numerical experiments.

## S17.02: Iterative methods

Date: March 19, 2026 08:30–10:30
Room: KII, M17.91
Chair(s): Schweitzer, Marcel

### Relaxation-Based Constructions of Algebraic Multigrid Methods

Kahl, Karsten; Moussa, Rayan 08:30
*Bergische Universität Wuppertal, Germany*

Algebraic Multigrid (AMG) methods are highly efficient solvers for large linear systems of equations, especially when classical iterative methods like Jacobi or Gauss-Seidel fail to converge quickly. By constructing a hierarchy of increasingly smaller problems whose combined solution approximates that of the original problem, multigrid methods are able to cheaply and efficiently eliminate the slow-to-converge components of the error.
Standard AMG approaches work by examining the static algebraic properties of the system matrix, A, to automatically construct the hierarchy of problems used in order to efficiently eliminate the error. However, as the error is a dynamic quantity that changes at each step and whose evolution is not governed by the problem matrix A iself, but rather by the relaxation operator $M^{-1}A$, it is more natural to approach the algebraic construction and analysis of AMG methods based on the relaxation method and its dynamical operator $M^{-1}A$, rather than the original static operator A.

Building on this idea, we introduce a novel systematic framework for developing multigrid techniques that fundamentally and solely relies on the dynamics of the relaxation process. By conceptualizing the relaxation process as a local discrete-time dynamical system mapped onto a spatio-temporal graph, we present a dynamical renormalization technique that facilitates the creation of a local non-Markovian interpolation process derived entirely from the dynamics of the relaxation method itself. Moreover, this refined approach to interpolation enables the formulation of more precise coarse equations, preserving the dynamical relations between the coarse points as faithfully as possible within the limits of locality.

In this talk, we will focus on a theoretical discussion of the core principles of this method, showcasing the derivation of the enhanced interpolation and coarse equations and their significant links to concepts such as compatible relaxation, ideal interpolation, ideal restriction and optimal interpolation.

### Grassmannian Flows and Near-Optimal Relaxation-Based Algebraic Multigrid

Moussa, Rayan; Kahl, Karsten 08:50
*University of Wuppertal, Germany*

Algebraic Multigrid (AMG) methods are highly effective algorithms for solving large linear systems of equations involving sparse critical operators, ones for which traditional iterative schemes (such as Jacobi, Gauss-Seidel, etc...) do not converge sufficiently well.
Conventional multigrid methods employ a hierarchy of increasingly coarser representations of the critical operator to tackle the various length-scales involved in its inversion process via appropriate local relaxation methods. The fundamental elements in the construction of such methods are the transfer operators which define the intricate connections between the various representations of the problem at hand. However, to ensure the efficiency of the overall method, it is necessary to enforce strong sparsity constraints on the transfer operators, ones which often interfere with the information encoded within, thus limiting the complementarity between the relaxation method in use and the coarse system we construct afterwards, often decreasing the efficiency of the resulting multigrid method.
In an attempt to overcome these limitations, we construct an alternative multigrid approach,

one which derives completely from the local relaxation method in use, meaning that the complementarity between it and the coarse system is explicitly ensured at the level of the fundamental multigrid equations, rather than implicitly through the transfer operators. We argue that an efficient application of such a multigrid formulation can take the form of a pseudo unigrid-like approach which employs a subspace flow on the Grassmanian manifold, one which is equivalent to a proper multilevel method corresponding to near-optimal interpolation operators albeit taking place almost entirely on the finer scales. As an example, we illustrate the application of such an approach on the Dirac equation of Lattice Quantum Chromodynamics (LQCD), and compare it's effect on the spectrum of the critical Dirac operator, its convergence behavior and the overall complexity of the setup and solve phases as compared to those of conventional AMG.

**Symbol-Based Analysis of Multigrid Methods for Maxwell's Equations on Structured Grids**

Spoerer, René; Bolten, Matthias 09:10
*Bergische Universität Wuppertal, Germany*

Discretising Maxwell's equations on structured grids yields linear systems with a multilevel block-Toeplitz structure. These structured matrices can be represented by a matrix-valued generating symbol, which we exploit to analyse the convergence of multigrid methods for these systems.

The large null space of the curl operator poses a significant challenge, necessitating careful asymptotic analysis of the differential operator's lower-order terms. In particular, the relationship between the smoother and coarse grid correction — the two fundamental building blocks of a multigrid method — depends on the discretisation step size. However, because the system's structure is preserved on coarser levels within this symbol-based framework, our convergence analysis remains independent of the number of levels employed.

Although we focus on systems arising from Nédélec finite elements, the analysis relies only on properties of the generating symbol rather than on the underlying function spaces. This enables straightforward extension to other discretisations, such as the finite integration technique.

**A new concept of block diagonal dominance and its application in randomized relaxations**

Frommer, Andreas (1); Szyld, Daniel (2) 09:30
*1: Bergische Universität Wuppertal, Germany*
*2: Temple University, Philadelphia, PA, USA*

For a linear system $Ax = b$, standard relaxation is equivalent to the Gauss-Seidel method and it convreges to the solution for any starting vector if $A$ is symmetric and positive definite or diagonally dominant by rows or columns. This result also holds for randomized relaxations, where the component to be relaxed is chosen randomly in each step.

In this talk we consider the generalization to block relaxation, and we allow the blocks to possibly overlap as is often the case in Schwarz type domain decomposition methods. Our main new contribution is a convergence result for serial and randomized block relaxations when $A$ fulfills an appropriate new generalization of diagonal dominance (by rows or by columns) to blocks.

**Exploiting Task-Based Parallelism for the Red-Black Gauss-Seidel Method on 2D Grids**

Long, Shiting (1); Ramirez-Hidalgo, Gustavo (2); Jimenez-Merchan, Jose (3); Frommer, Andreas (3); Pleiter, Dirk (1,4) 09:50
*1: KTH Royal Institute of Technology, Sweden*
*2: Forschungszentrum Jülich GmbH, Germany*
*3: University of Wuppertal, Germany*
*4: University of Groningen, Netherlands*

Gauss–Seidel is a well-established iterative method for the solution of linear systems, and multicoloring has been widely used to increase parallelism in iterative solution techniques. Implementing multicolor Gauss–Seidel with conventional divide-and-conquer parallelization strategies, however, may be inefficient due to global synchronization requirements and load imbalances. Task-based programming models can mitigate these issues by enabling fine-grained parallelism, removing global barriers

and allowing updates of different colors to partially overlap in time. This structure may also improve cache reuse, as the task scheduler can update nearby grid points shortly after one another. While cache-aware Gauss–Seidel variants exist, task-based models provide a simpler and more flexible way to realize the benefits.

In this work, we implement a red–black Gauss–Seidel method using task-based programming paradigms and evaluate it against a classical divide-and-conquer implementation to assess the impact of fine-grained parallelism on execution efficiency. The red–black scheme is chosen as a representative example, as the task-based approach readily extends to general multi-color schemes, including those arising from unstructured grids or wider stencils. We focus on the 2D Poisson equation as our primary benchmark.

**A matrix based analysis of the non-Hermitan Lanczos Algorithm**

Liesen, Jörg; Ramme, Justus
*Technische Universität Berlin, Germany*

10:10

In 1950, Lanczos published a fundamental algorithm that reduces a given non-Hermitian matrix to tridiagonal form using two coupled three-term recurrences, which produce two sequences of biorthogonal vectors. A major issue with this algorithm is that it can experience so-called serious breakdowns. The intriguing behavior of the algorithm and its breakdowns has since motivated numerous analyses from many different mathematical viewpoints.
In this talk, we will present a new and entirely matrix based analysis of the algorithm that transparently explains its "mechanics", the causes of all possible types of breakdowns, and the "look-ahead technique" that was devised to deal with serious breakdowns. We will revisit important mathematical results about the algorithm, such as Taylor's Mismatch Theorem, and present some new results. Moreover, we will discuss properties and possible simplifications of the algorithm for several special matrix classes, in particular H-selfadjoint matrices.
The talk is based on joint work with Jörg Liesen (TU Berlin).

## S17.03: Approximate computing

Date: March 19, 2026 14:00–16:00
Room: KII, M17.91
Chair(s): Tabeart, Jemima

**Least squares problems: accurate solutions with approximate computing**

Meier, Maike (1); Epperly, Ethan N. (2); Lister, Andrew (3); Nakatsukasa, Yuji (4); Scott, Jennifer (3)
*1: University of Groningen, Netherlands, The*
*2: UC Berkely, USA*
*3: University of Reading and STFC Rutherford Appleton Laboratory, UK*
*4: University of Oxford, UK*

14:00

Large linear least squares (LS) problems are ubiquitous in scientific computing. In recent years, there has been a boom in interest for techniques that offer fast but accurate solutions to enormous problems. Two popular directions for new solvers are 1) the introduction of randomized elements, and 2) the introduction of multiple precisions. Both elements introduce a certain inaccuracy in computations, but offer big speed-ups for large problems. In fact, one of the greatest success stories of randomized algorithms for linear algebra has been the development of fast, randomized algorithms for highly overdetermined LS problems, such as sketch-and-solve and sketch-and-precondition. Similarly, a variety of mixed-precision iterative refinement-based solvers have been introduced in recent years, aiming to leverage hardware development that increases the efficiency of mixed-precision computations. In this talk, we discuss various recent algorithms with 'approximate computing' techniques and pay particular attention to the question: how can we still compute highly accurate solutions?

**Reduced and Mixed Precision Householder QR Decomposition**

Benner, Peter; Koehler, Martin; Liu, Xiaobo; Oktay, Eda
*Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg, Germany*

14:40

Recent advances in hardware architectures have highlighted the importance of reduced-precision arithmetic for improving performance and lowering energy consumption in large-scale scientific applications. However, uniformly low-precision methods can suffer from numerical instability, especially in fundamental linear algebra routines. Mixed-precision strategies, therefore, play a crucial role in balancing efficiency, stability, and accuracy.
In this talk, we focus on the Householder QR decomposition using the WY representation and explore its behavior under reduced- and mixed-precision settings. We first present a uniform half-precision implementation and evaluate its potential performance benefits and significant numerical-accuracy limitations. We then show how increasing the precision of selected computations within the algorithm can substantially improve stability and analyze how these precision choices impact overall performance.

**A general framework for Krylov ODE residuals with applications to randomized Krylov methods**

Krieger, Emil; Schweitzer, Marcel
*Bergische Universität Wuppertal, Germany*

15:00

Randomized Krylov subspace methods that employ the sketch-and-solve paradigm to substantially reduce orthogonalization cost have recently shown great promise in speeding up computations for many core linear algebra tasks (e.g., solving linear systems, eigenvalue problems and matrix equations, as well as approximating the action of matrix functions on vectors) whenever a nonsymmetric matrix is involved. An important application that requires approximating the action of matrix functions on vectors is the implementation of exponential integration schemes for ordinary differential equations. In this paper, we specifically analyze randomized Krylov methods from this point of view. In particular, we use the residual of the underlying differential equation to derive a new, reliable a posteriori error estimate that can be used to monitor convergence and decide when to stop the iteration. To do so, we first develop a very general framework for Krylov ODE residuals that unifies existing results, simplifies their derivation and allows extending the concept to a wide variety of methods beyond randomized Arnoldi (e.g., rational Krylov methods, Krylov methods using a non-standard inner product, ...). In addition, we discuss certain aspects regarding the efficient implementation of sketched Krylov methods. Numerical experiments on large-scale ODE models from real-world applications illustrate the quality of the error estimate as well as the general competitiveness of sketched Krylov methods for ODEs in comparison to other Krylov-based methods.

**Bridging continuous and discrete tensor formats of multivariate functions via QTT**

Benner, Peter (1); N. Khoromskij, Boris (1,2); Sun, Bonan (1)
*1: Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstr. 1, D-39106 Magdeburg, Germany*
*2: Max Planck Institute for Mathematics in the Sciences, Inselstr. 22-26, D-04103 Leipzig, Germany*

15:20

Continuous (functional) low-rank tensor formats of multivariate functions have gained lots of attention recently. These formats approximate $f : [-1, 1]^d \to \mathbb{R}$ as a rank-structured separable summation of univariate functions and numerical coefficients. In this work, we focus on the Chebyshev-Tucker format [1]

$$f(x_1, \dots, x_d) \approx \sum_{j_1=1}^{r} \cdots \sum_{j_d=1}^{r} \boldsymbol{\beta}_{j_1,\dots,j_d} v_{j_1}^{(1)}(x_1) \cdots v_{j_d}^{(d)}(x_d),$$

a functional Tucker format with core $\boldsymbol{\beta} \in \mathbb{R}^{r\times\cdots\times r}$ and univariate functions parametrized in a Chebyshev basis $v_{j_\ell}^{(\ell)}(x_\ell) = \sum_{k=0}^{m} V_{k+1,j_\ell}^{(\ell)} T_k(x_\ell)$ of degree at most $m$.
Many numerical methods, in contrast, are substantiated via grid-based representations, where the function $f$ is discretized on a fine $n^{\otimes d}$ tensor product grid and identified with a tensor $\mathbf{F} \in \mathbb{R}^{n\times\cdots\times n}$

of function values at the grid points. To remain computationally feasible, $\mathbf{F}$ is thus also sought in a discrete low-rank tensor format. Transforming continuous to discrete low-rank formats is therefore a natural task. The naive approach is to directly evaluate the polynomials $v_{i_\ell}^{(\ell)}(x_\ell)$ at the grid points, yielding a discrete Tucker tensor with factor matrices $U^{(\ell)} \in \mathbb{R}^{n\times r}$. However, this is prohibitively expensive on fine grids, requiring $\mathcal{O}(dnr)$ storage.

We propose to instead discretize the polynomials $v_{i_\ell}^{(\ell)}(x_\ell)$ in the Quantized Tensor Train (QTT) format [4]. The resulting tensor $\mathbf{F}$ admits a two-level QTT-Tucker-like format [3], where each column of the factor matrices $U^{(\ell)}$ is represented compactly in the QTT format. For this purpose, we introduce and analyze novel algorithms for computing QTT approximations of univariate functions with guaranteed accuracy without forming the full $n$-point discretization. This method outperforms existing methods based on TT adaptive cross procedures in both accuracy and efficiency and is of broader interest. Numerical experiments show the $\varepsilon$-numerical QTT ranks scale logarithmically with $m$, so the Tucker factor matrices require only $\mathcal{O}(dr\log^2 m\log n)$ storage. Finally, we demonstrate the resultant discrete QTT-Tucker representation recovers, with high accuracy and reduced storage, earlier results on grid-based low-rank tensor methods for electrostatic potential of multi-particle systems. This is based on joint work with P. Benner and B. N. Khoromskij [2].

[1] P. Benner, B. N. Khoromskij, V. Khoromskaia, and B. Sun. A mesh-free hybrid Chebyshev-Tucker tensor format with applications to multi-particle modelling. arXiv:2503.01696, 2025.

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**Computation of low rank approximations of matrix polynomials using regularization**

Enerbäck, Jenny; Dmytryshyn, Andrii; Strömberg, Ann-Brith 15:40

*Chalmers University of Technology, Gothenburg University, Sweden*

Polynomial eigenvalue problems are a well-known and extensively studied problem in mathematics. Theories and tools developed to solve these problems are among the most important contributions of mathematics to technology, engineering, and physics. However, novel developments in modern technology and advanced engineering increasingly require accurate and efficient solutions to new and challenging eigenvalue problems, e.g, singular eigenvalue problems (originating from low-rank approximations or involving rank-deficient structures due to the modeling techniques employed). Applying standard methods designed for nonsingular cases to singular problems can lead to catastrophic errors—computed eigenvalues may be entirely incorrect, dominated by round-off effects. Moreover, existing tools typically cannot provide warning that the results may be unreliable.

Introducing a singularity check before solving an eigenvalue problem may not be enough to determine the reliability of the results, since small perturbations, coming from uncertainties in data or round-off errors, almost always transform a singular problem to a nonsingular problem. Consequently, a robust way to evaluate reliability of the computations is itself a challenging problem. One way to tackle it is computing a distance to singularity, i.e., the norm of the smallest perturbation that will make our problem singular. Recently a few algorithms, relying on completely different ideas, were developed to compute this distance but the problem remains challenging, in particular, for the polynomials of large size.

In the presentation, we propose a new algorithm for approximating a given matrix polynomial with another matrix polynomials of rank at most *r* and also compute the distance from this given matrix polynomial to the computed approximation. Note that the "distance-to-singularity" problems is included here when the rank is chosen to be one less than the size. We use regularization techniques and build on a recently developed algorithm which in turn is using generic eigenstructures, their parametrizations, and an alternating least squares scheme. In a similar way, we also cover the case of skew-symmetric matrix polynomials.

In preliminary tests, our algorithm is typically faster than the state–of–the–arts methods, while showing a similar accuracy, for both the skew-symmetric and general problems. This allows us to handle problems of larger size, as well as multiple starting guesses for small–to–medium size problems.

## S17.04: Other topics in applied and numerical linear algebra

Date: March 20, 2026 08:30–10:30
Room: KII, M17.91
Chair(s): Tabeart, Jemima

### A novel graph coloring technique for the trace estimation of an inverse Dirac matrix

Papace, Mario (1); Frommer, Andreas (1); Jimenez-Merchan, Jose (1); Lang, Bruno (1); Ramirez-Hidalgo, Gustavo (2) 08:30
*1: Bergische Universität Wuppertal, Germany*
*2: Jülich Supercomputing Centre, Germany*

The evaluation of the trace of the inverse of a large, sparse matrix $A$ is a fundamental problem in many areas of computational science, most notably in Lattice Quantum Chromodynamics (LQCD), where the trace of the inverse of the Wilson-Dirac matrix is essential for many calculations. A common strategy is to represent the trace as the expected value of matrix quadratures and approximate it using Monte Carlo sampling. While this stochastic approach is widely used, its effectiveness is often limited by high variance, since random test vectors fail to exploit the structural decay properties typically exhibited by $A^{-1}$ away from the sparsity pattern of $A$. Probing offers an effective variance-reduction strategy by constructing deterministic vectors, known as probing vectors, that are tailored to the sparsity structure of $A$. When such decay of $A^{-1}$ entries from the sparsity pattern of $A$ is exhibited, the key idea is to interpret $A$ as the adjacency matrix of a graph and apply distance-$d$ graph coloring techniques to partition rows and columns into structurally independent sets. When probing is combined with stochastic estimators such as Hutchinson's method, the result is a hybrid framework that substantially reduces variance and improves reliability in trace approximation. This combination has proven particularly powerful in applications involving large-scale sparse matrices. In this talk, we will present the theoretical principles underlying probing, based on a novel graph coloring technique and compare it to already existing coloring frameworks. Furthermore, we will describe how probing can be combined with stochastic trace estimation methods, and illustrate its application to the estimation of physical observables in LQCD and the resulting gains in accuracy, variance reduction, and computational efficiency.

### A Two-Phase Approach to Distance-d Coloring of Grids and Tori

Lang, Bruno 08:50
*University of Wuppertal, Germany*

A distance-$d$ coloring of a graph assigns a color to each node such that all nodes at distance $\leq d$ have different colors. Such colorings can be used to decouple quantities for exploiting parallelism, and for reducing variation in stochastic estimators, e.g. for the trace of the inverse of a sparse matrix in Lattice QCD computations. In the latter application, the graph typically is a three- or four-dimensional torus, and a small number of colors is desirable to reduce overall work. In addition, the coloring should parallelize well, which is guaranteed if the color of a node depends only on its position within the torus. So far, a hierarchical algorithm has been employed to achieve this for power-of-two distances $d = 2^D$.
We present a two-phase approach to determine parameters $\sigma_1, \ldots, \sigma_d$ such that the coloring given by $c(x) = ( \sum_j \sigma_j x_j ) \bmod n_c$ indeed is a distance-$d$ coloring of the torus. Here, $c(x)$ denotes the color of a node at position $x = (x_1, \ldots, x_d)$, and $n_c$ is the number of colors. The first phase tries to find an initial feasible combination $(\sigma_1, \ldots, \sigma_d)$ and thus establishes bounds for the $\sigma_j$, which are used in the second phase to search for combinations with a lower number of necessary colors. Our approach typically reduces the number of colors considerably, as compared to the hierarchical algorithm. In practice, we often achieve $n_c \leq 2\, \chi_d$, where $\chi_d$ is the chromatic number of the distance-$d$ graph, i.e.,

the lowest possible number of colors. In addition, our coloring scheme is not restricted to power-of-two distances.

**Certified Model Order Reduction for parametric Hermitian eigenproblems**

Manucci, Mattia; Stamm, Benjamin; Zeng, Zhuoyao 09:10
*University of Stuttgart, Germany*

We deal with the efficient and certified numerical approximation of the smallest eigenvalue and the associated eigenspace of a large-scale parametric Hermitian matrix. For this aim, we rely on projection-based model order reduction (MOR), i.e., we approximate the large-scale problem by projecting it onto a suitable subspace and reducing it to one of a much smaller dimension. Such a subspace is constructed by means of weak greedy-type strategies.
After detailing the connections with the reduced basis method for source problems, we introduce a novel error estimate for the approximation of the eigenspace associated with the smallest eigenvalue. Since the difference between the second smallest and the smallest eigenvalue, the so-called spectral gap, is crucial for the reliability of the error estimate, we propose efficiently computable upper and lower bounds for higher eigenvalues and for the spectral gap, which enable the assembly of a subspace for the MOR approximation of the spectral gap.
Based on that, a second subspace is then generated for the MOR approximation of the eigenspace associated with the smallest eigenvalue. We also provide efficiently computable conditions to ensure that the multiplicity of the smallest eigenvalue is fully captured in the reduced space. This work is motivated by a specific application: the repeated identifications of the states with minimal energy, the so-called ground states, of parametric quantum spin system models.

**Optimal Damping for the 1D Wave Equation Using a Single Damper**

Mlinaric, Petar (1); Gugercin, Serkan (2); Tomljanovic, Zoran (3) 09:30
*1: Department of Mathematics, Faculty of Science, University of Zagreb, Croatia*
*2: Department of Mathematics and Division of Computational Modeling and Data Analytics, Academy of Data Science, Virginia Tech, USA*
*3: School of Applied Mathematics and Informatics, University of Osijek, Croatia*

Vibrational structures are susceptible to catastrophic failures or structural damage when external forces induce resonances or repeated unwanted oscillations. One common approach is to use dampers to suppress these disturbances. This leads to the problem of finding optimal damper viscosities and positions for a given vibrational structure. Although extensive research exists for finite-dimensional systems, optimizing damper positions remains challenging due to their discrete nature.

To overcome this, we introduce a novel model for the damped wave equation (at the PDE level) with a damper of viscosity **v** at position **p**, and develop a system-theoretic, input–output–based analysis in the frequency domain. In this formulation, we consider the average displacement as the output, while for the input (forcing) we analyze two cases: uniform forcing and boundary forcing. For both cases, explicit formulas are derived for the corresponding transfer functions, parametrized by **p** and **v**.

This explicit parametrization facilitates the analysis of the optimal damping problem (at the PDE level) using norms such as the $H_2$ and $H_\infty$ norms. We also examine limiting cases, such as very large viscosity or the absence of external damping. To illustrate our approach, we present numerical examples, compare different optimization criteria, and discuss the impact of damping parameters on the damped wave equation.

**Structured stability radii for linear Dissipative-Hamiltonian systems.**

Benner, Peter (1); Mehrmann, Volker (2); Prajapati, Anshul (1); Sharma, Punit (3) 09:50
*1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
*2: Institute of Mathematics, TU Berlin, Germany*
*3: Department of Mathematics, IIT Delhi, India*

We study linear time-invariant Dissipative Hamiltonian (DH) systems arising in energy-based modeling of dynamical systems. An advantage of DH systems is that they are always stable due to the structure of their coefficient matrices, and, under further weak conditions, even asymptotically stable. Here, we consider the computation of the stability radii for a given asymptotically stable DH system; i.e., the smallest structured perturbation that puts a DH system on the boundary of the region of asymptotic stability, so that it has purely imaginary eigenvalues. We obtain explicit computable formulas for various structured stability radii. For this, the problem of computing stability radii is reformulated in terms of minimizing the Rayleigh quotient of a Hermitian matrix or the sum of two generalized Rayleigh quotients of Hermitian semidefinite matrices. This reformulation results in the problem of minimizing the largest eigenvalue of an eigenvector-dependent Hermitian matrix or minimizing the smallest eigenvalue of a Hermitian matrix that depends on the eigenvector. We then demonstrate (via numerical experiments) that, under structure-preserving perturbations, the asymptotic stability of a DH system is much more robust than under general perturbations, since the distance to instability is typically much larger when structure-preserving perturbations are considered.

**ResQPASS: Generalising Krylov subspace methods to solve constrained linear least squares problems**

Symoens, Bas; Vanroose, Wim 10:10
*Univeristy of Antwerp, Belgium*

Large-scale constrained linear least squares problems are foundational in applications like mechanics with contact, image reconstruction, and sparse data science. While Krylov subspace methods are well studied and highly efficient for the unconstrained case, they cannot handle constraints directly. We present the Residual Quadratic Programming Active Set Subspace (ResQPASS) method, which synthesizes active set strategies with key concepts of Krylov subspaces to solve these constrained problems efficiently. ResQPASS preserves a key strength of Krylov methods: when all constraints are inactive, it reduces to the standard LSQR algorithm, and it maintains Krylov-like asymptotic convergence for the constrained case.

The algorithm requires only matrix-vector products, vector updates, and inner products, ensuring scalability. Its practical performance is enhanced through warm-starting, solving intermediate subproblems inexactly, and maintaining a factorisation updated via efficient rank-one updates. Depending on the structure of the problem, users can use the primal formulation (optimal when few constraints are active) or the dual formulation (preferable when many constraints are active). Consequently, ResQPASS provides a framework that bridges the gap between established Krylov solvers and the demands of constrained optimization.

## S18: Numerical methods for differential equations

Organizer(s): Haubold, Tim *(Georg August Universität Göttingen)*
Wick, Thomas *(Leibniz University Hannover)*

## S18.01: Space-time and goal-oriented error control

Date: March 17, 2026 08:30–10:30
Room: KI, M11.71
Chair(s): Steinbach, Olaf
Bause, Markus
Wick, Thomas

### On space-time analysis of parabolic problems on tensor product meshes

Löscher, Richard; Reichelt, Michael; Steinbach, Olaf
*TU Graz, Austria*
08:30

In this talk, we focus on parabolic initial–boundary value problems with varying regularity of the initial data. As is well known for time-stepping methods, rough initial data can lead to oscillations in the finite element solution and therefore requires adapted strategies, such as geometric warm-up or mixed time-stepping schemes. We discuss space–time variational formulations that incorporate the initial data in both a strong and an ultra-weak sense in time. On tensor-product space–time meshes, we derive finite element error estimates that highlight the advantages and limitations of each formulation. Numerical examples complement the theoretical results.

### A Space-Time Finite Element Method for the Stokes System on Simplicial Meshes

Kaltenbacher, Tobias; Steinbach, Olaf
*Graz University of Technology, Austria*
08:50

In this talk, we consider a space-time finite element method for the time-dependent Stokes system. While classical approaches rely on time-stepping schemes, we propose a fully space-time variational formulation in the Bochner space setting. We first study the formulation on tensor-product space-time meshes and then extend it to completely unstructured space-time meshes, allowing for a unified treatment of spatial and temporal discretization. Numerical experiments on arbitrary space-time meshes illustrate the flexibility and effectiveness of the proposed approach.

### Analysis of a Non-Symmetric Space-Time FEM-BEM Coupling for a Parabolic-Elliptic Transmission Problem

Kaltenbacher, Tobias; Of, Guenther
*Graz University of Technology, Austria*
09:10

We study a transmission problem coupling the heat equation in a bounded Lipschitz domain with the Laplace equation in the exterior domain. A space-time formulation of the heat equation is coupled with the weakly singular boundary integral equation of the Laplace equation. We provide a complete analysis of the resulting space-time formulation. Furthermore, we introduce a conforming discretization, analyze the corresponding discrete variational problem, and discuss the implementation of the resulting FEM-BEM coupling. Finally, we present numerical experiments that are in agreement with the theoretical results.

### Goal-Oriented Adaptivity and Multigrid Techniques for Flow Problems

Bruchhäuser, Marius Paul (1); Bause, Markus (1); Margenberg, Nils (2)
*1: Helmut Schmidt University Hamburg, Germany*
*2: Otto von Guericke University Magdeburg*
09:30

The Dual Weighted Residual (DWR) Method has attracted researchers' interest in many fields of application problems since it was introduced by Becker and Rannacher at the turn of the last millennium.

With regard to an efficient numerical approximation of the underlying model problem, the DWR approach yields an a posteriori error estimator measured in goal quantities of physical interest, that can be used for adaptive mesh refinement in space and time. Here, we apply this goal-oriented error control in combination with efficient iterative solver technologies to nonstationary Navier-Stokes equations. More precisely, a generalized minimal residual (GMRES) method using a geometric multigrid (GMG) method as a preconditioner is applied to the resulting linear system within Newton's method. The performance properties of the underlying algorithm are studied by means of well-known benchmarks for nonstationary flow problems. Moreover, an outlook to the extansion of anisotropic mesh refinement is given, evidenced by some numerical examples.

**A Goal-Oriented Error Estimation Framework for Thermodynamic Topology Optimization using Adaptive Virtual Elements**

Sellmann, Christian; Wick, Thomas; Junker, Philipp 09:50
*Leibniz Universität Hannover, Germany*

In this talk, we present a fully adaptive topology optimization framework for 2D and 3D applications, utilizing the goal-oriented dual-weighted residual (DWR) a posteriori error estimation method.
The mechanical problem is solved using the Virtual Element Method (VEM), which facilitates straightforward mesh refinement while allowing for a computationally efficient approximation of the DWR error. In the proposed framework, elements are marked based on both the local element error and changes in the density field. This approach results in an efficient adaptive process that avoids the introduction of heuristic hyperparameters.
Numerical results demonstrate that the adaptive framework produces the same final structures as a uniform fine mesh but at a significantly reduced computational cost. We investigate the properties of the scheme through various benchmarks to validate its performance and accuracy.

**Anisotropic Goal Oriented hp-Adaptivity for Time-dependent Problems**

Bause, Markus (2); Bruchhäuser, Marius Paul (2); Endtmayer, Bernhard (1); Margenberg, Nils (3); Toulopoulos, Ioannis (4); Wick, Thomas (1) 10:10
*1: Leibniz University Hannover, Germany*
*2: Helmut Schmidt University Hamburg, Germany*
*3: Otto-von-Guericke-Universität Magdeburg, Germany*
*4: University of Western Macedonia, Greece*

In this talk, we introduce an anisotropic goal-oriented hp-adaptivity based on the Dual Weighted Residual (DWR) method. The presented approach leverages p-anisotropic finite element spaces, enabling the elementwise separation of spatial and temporal directions to naturally induce adaptive, anisotropic refinement. This allows to use full hp-adaptivity, which can resolve very sharp layers arising from convection dominated problems. Finally the numerical experiments are backened by numerical examples.

## S18.02: Cut and unfitted finite elements

Date: March 17, 2026 16:30–18:30
Room: KI, M11.71
Chair(s): Wick, Thomas

**A Cut Finite Element Method for Fully Eulerian Fluid-Structure Interaction**

Frei, Stefan (1); Knoke, Tobias (2); Steinbach, Marc (2); Wenske, Ann-Kathrin (2); Wick, Thomas (2) 16:30
*1: University of Konstanz, Germany*
*2: Leibniz Universität Hannover*

A Eulerian description of fluid-structure interactions (FSI) is convenient in case of large structural deflections or if the solid might come into contact with itself or with other solid bodies. One major diffulty for the discretisation of fully Eulerian FSI is the fact that the interface between fluid and solid moves over the computational domain. Using a standard time-stepping scheme, this means that mesh cells might change their domain affiliation over time and are cut in different portions at each time step.

In this talk, we present a cut finite element approach that takes care of these issues. Thereby, the fluid-solid-coupling is included weakly by means of Nitsche's method and a ghost penalty stabilisation is applied to guarantee robustness of the method, independently of the way the interface cuts through mesh cells. We use inf-sup stable finite elements in the fluid and a first-order-in-time velocity-displacement formulation for the solid on quadrilateral meshes, in combination with a backward-Euler type time-stepping scheme. Optimal-order convergence estimates in space and time can be shown for the case of a linear fluid-structure interaction problem under the assumption of a fixed interface. Finally, the numerical method is investigated by means of detailed numerical tests, including the fall and bounce of an elastic ball within a viscous fluid.

**A linear fluid-structure interaction problem using CutFEM: Numerical Analysis**

Frei, Stefan (1); Knoke, Tobias (2); Steinbach, Marc (2); Wenske, Anne-Kathrin (2); Wick, Thomas (2)
*1: University of Konstanz, Germany*
*2: Leibniz Universität Hannover, Germany*

16:50

Geometrically unfitted finite element methods such as CutFEM have been studied and applied to problems where resolving geometries is unfavourable. For example in fluid-structure interaction problems, using an Eulerian description for both subproblems allows the derived method to handle large deformations, topology changes and contact problems more easily, while the interface between fluid and structure will not be resolved by the computational mesh.

Previously, a CutFEM approach together with Ghost Penalties based on jump terms has been applied succesfully to this type of fully Eulerian fluid-structure interaction problems. For a linear problem with artificially fixed interface optimal convergence rates have been shown numerically.

In this talk, we will expand on the numerical analysis of the linear fluid-structure interaction problem. We discuss stability estimates of the underlying bilinear form as well as L2-L2-pressure stability due to the use of inf-sup-stable finite elements in the fluid. Finally, we derive optimal a priori error estimates.

**Homogenization and XFEM for Interface-resolved Diffusion in Complex 3D Microstructures**

Puderbach, Janna
*Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany*

17:10

The cathode of a solid oxide fuel cell (SOFC) has a highly complex three-dimensional microstructure. Ion exchange across material interfaces leads to discontinuities in the solution of a diffusion problem, while the complicated geometry of the microstructure causes highly oscillatory solution behavior. The accurate resolution of these effects in three dimensions poses significant challenges for computation and meshing.
To solve this, we use an asymptotic expansion technique to derive a homogenized model that avoids the need for explicit resolution of the entire microstructure. The resulting multiscale formulation consists of a microscopic cell problem that captures local behavior and a macroscopic problem that determines the global response. The effectiveness of the homogenized model is demonstrated by a quantitative comparison with the fully resolved microscopic solution.
To accurately handle solution discontinuities at material interfaces in the three dimensional microscopic problem while avoiding complex geometry conforming mesh generation, we employ the extended finite element method (XFEM). This approach enables precise interface resolution while significantly reducing mesh complexity and is therefore well suited for multiscale simulations of realistic SOFC microstructures.

**Stabilized finite element methods for incompressible (Navier-)Stokes flows on a family of curved surfaces**

Kaiser, Michael Wolfgang; Fries, Thomas-Peter
*Graz University of Technology, Austria*

17:30

Residual-based stabilization techniques for finite element methods are presented for the simulation of incompressible (Navier-)Stokes flows on curved surfaces. The surfaces on which the flows take place may be considered individually or simultaneously as a family of surfaces which are embedded

in a three dimensional bulk domain. For the numerical solution, this leads to the classical Surface FEM for single surfaces [1] or to the Bulk Trace FEM for the simultaneous analysis [2]. In both cases, the inf-sup condition results from the mixed formulation in velocity and pressure variables which has to be considered in the applied numerical method. To handle this in a finite element context, one may use Taylor-Hood elements, e.g., [1,2], or equal-order element pairs for velocity and pressure together with a stabilization scheme, e.g., the Brezzi-Pitkäranta stabilization [3] or the PSPG method [4]. Herein, the formulation of the PSPG method [4] for classical Euclidean geometries is extended to (Navier-)Stokes flows on curved surfaces to enable consistent equal-order approximations. A crucial aspect for flow problems on surfaces is the consideration of the tangential velocity in the governing equations, e.g., [1–3,5]. This modelling aspect significantly influences the formulation of the residual-based stabilization techniques. A model with a projection of the velocity field onto the tangent space of the manifold, see, e.g. [3,5], is used here. Results obtained with PSPG and equal-order element pairs for velocity and pressure are compared to inherently stable solutions computed with Taylor-Hood elements. Furthermore, a numerical inf-sup test is presented to verify the stabilized finite element methods.

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**Phase-Field Model for Nonisothermal Melt Flow: Structure-Preserving Approximation**

Brunk, Aaron; Höhn, Dennis 17:50
*Johannes-Gutenberg University Mainz, Germany*

In this talk, we present a nonconserved phase-field model for describing melt-flow dynamics in a nonisothermal, two-phase solid–liquid mixture. The governing system of partial differential equations consists of an Allen–Cahn-type equation for the phase field, a heat-transfer equation formulated in terms of internal energy or entropy, and the incompressible Navier–Stokes equations to capture the fluid flow. We develop suitable weak formulations that preserve fundamental thermodynamic principles, such as energy conservation and entropy production. These properties carry over to the fully discrete finite element approximation, which employs a problem-adapted Petrov–Galerkin time discretization. Finally, we demonstrate the effectiveness of the proposed numerical scheme through convergence studies and illustrative examples.

**Parameter-robust unfitted finite element methods for a Maxwell interface problem**

Haubold, Tim; Lehrenfeld, Christoph 18:10
*Georg August Universität Göttingen, Germany*

Geometrically unfitted finite element methods such as CutFEM, Finite Cell, XFEM or unfitted DG methods have been developed and applied successfully in the last decades to a variety of problems, ranging from scalar PDEs on stationary domains to systems of PDEs on moving domains and PDEs on level set surfaces. These approaches combined with established tools of finite element methods allowed to apply and analyse unfitted methods in many fields. In this talk, we deal with an elliptic interface problem for the time-harmonic quasi-magnetostatic Maxwells equations. Here the material function $\mu$, the magnetic permeability, can jump at an interface. Such problems

are considered in low-frequency applications. Standard unfitted Nitsche methods are not robust with respect to the parameter k, proportional to the wavenumber. For example, a standard Nitsche discretization for the curl-curl-operator introduces terms that do no longer vanish for gradient fields.
In this talk, we will use a vectorial finite element discretization based on H(Curl) conforming functions. We will tackle the problem of robustness by using a mixed formulation and a Nitsche formulation. Additionally, we apply a careful tailored ghost penalization term. We will also give a short discussion of possible preconditioners.

## S18.03: Least squares methods

Date: March 18, 2026 08:30–09:30
Room: KI, M11.71
Chair(s): Wick, Thomas

### A certified reduced order model for parabolic equations based on a least-squares space time formulation

Hinze, Michael (1); Kahle, Christian (2); Michael, Stahl (3) 08:30
*1: Universität Koblenz, Germany*
*2: Universität Koblenz, Germany*
*3: Universität Koblenz, Germany*

We propose a least-squares formulation for parabolic PDEs in the natural $L^2(0,T;V^*)xH$ norm which avoids regularity assumptions on the data of the problem, which e.g. appear in the recently proposed *First Order System Least Squares (FOSLS)* method. For abstract parabolic equations the resulting bilinear form then is symmetric, continuous, and coercive. This among other things paves the ground for classical space-time a priori and a posteriori Galerkin frameworks for the numerical approximation of this problem class.

The approach is applicable for parameterized parabolic equations as well and we introduce a model order reduction technique that takes over all advantages from well-known elliptic settings. We introduce a POD-greedy method in some space-time energy norm at hand with absolute and relative error bounds. Numerical examples illustrate the performance of the method.

### A Greedy Residual-Based Method for Kernel Collocation of Nonlinear PDEs

Bacchetta, Milan (1,2); Ehring, Tobias (1); Haasdonk, Bernard (1) 08:50
*1: University of Stuttgart, Germany*
*2: Universität des Saarlandes*

*Symmetric kernel collocation is a well-established meshless method for solving linear partial differential equations (PDEs). Recent work [1] has extended this framework to handle nonlinear PDEs. A central challenge in these methods is the optimal selection of collocation points to ensure efficiency and accuracy. Motivated by dimension-independent convergence rates proven for greedy methods in the linear setting [2], we propose a novel PDE-residual-driven greedy algorithm for point selection in the nonlinear case [3]. We present a theoretical analysis demonstrating that, under assumptions similar to those in [1], our method converges both in terms of the vanishing PDE residual and in the Reproducing Kernel Hilbert Space norm. Our numerical experiments corroborate the theory, showing that the proposed greedy strategy yields significantly faster convergence compared to fill-distance-based sampling for the same number of centres. This approach provides an adaptive, problem-dependent strategy for constructing efficient kernel approximations, where point selection is driven by the PDE residual itself.*
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**Least-Squares methods for eigenvalue problems**

Bertrand, Fleurianne 09:10
*TU Chemnitz, Germany*

Accurate flux approximations are of interest in many applications and this is particularly true for fluid-structure interaction problems. Considering the corresponding spectral problem, the Least-Squares method involves the flux and the stress as independent variables approximated in a suitable H(div)-conforming finite element spaces. This talk will discuss recent results on the applicability of the Least-Squares method for the determination of the corresponding elastoacoustic vibrations, and show that the resulting scheme provides a correct spectral approximation. Quasi-optimal error estimates and numerical experiments to confirm those will be provided.

## S18.04: Numerical analysis for PDEs

Date: March 18, 2026 14:00–16:00
Room: KI, M11.71
Chair(s): Haubold, Tim

**Pressure robustness for incompressible fluid flow with inhomogeneous Dirichlet boundary conditions**

Eickmann, Franziska (1); Scott, L. Ridgway (2); Tscherpel, Tabea (1) 14:00
*1: TU Darmstadt, Germany*
*2: University of Chicago (Emeritus), US*

Pressure robust mixed finite element methods have the advantage that, for the Stokes equations, the velocity error is independent of both the pressure best approximation error and the viscosity. This makes them particularly attractive for low-viscosity regimes and in situations of low pressure regularity. One way to achieve pressure robustness is the use of exactly divergence-free finite element methods, such as the Scott-Vogelius element. However, for non-compatible inhomogeneous Dirichlet boundary conditions, pressure-robustness may deteriorate.

In this talk, we present best approximation results for the Stokes equations without extra boundary error term for general inf-sup stable mixed finite elements spaces, together with the corresponding result for pressure-robust elements. Moreover, for the Scott-Vogelius method, we analyse the properties of a Uzawa type algorithm.

**Adaptive Mixed Finite Element Method for Stress-Based Formulations of Eigenvalue Problems**

Dağlı, Tugay; Bertrand, Fleurianne 14:40
*TU Chemnitz, Germany*

In this talk, we present a novel three-field mixed finite element method for eigenvalue problems (EVPs) arising in Stokes flow and linear elasticity. To this end, we approximate the Hellinger–Reissner formulation, in which the symmetry of the stress tensor is enforced weakly by introducing a Lagrange multiplier that represents the conservation of angular momentum. We consider a tensor-valued stress field with rows in a Raviart–Thomas space, a discontinuous piecewise-polynomial vector field for the velocity (in Stokes) or displacement (in elasticity), and a continuous piecewise-polynomial space for weakly imposing symmetry. This yields a stress–velocity–vorticity formulation for the Stokes EVP and a stress–displacement–rotation formulation for the linear elasticity EVP, both discretized with $RT_k^d - DP_k^d - P_k^{\frac{d(d-1)}{2}}, \quad k \geq 1,\ d \in \{2,3\}$. The formulation offers significant advantages, as it is derived directly from fundamental physical principles, including linear momentum balance, constitutive laws, and—specifically in the Stokes case—mass conservation. Moreover, it enables a direct approximation of the stress field, which is crucial in many applications. Finally, it allows for an efficient and

reliable a posteriori error estimator, and we incorporate an adaptive refinement strategy. This adaptive procedure enables the recovery of optimal convergence rates even in the presence of singularities in the solution. Numerical experiments on convex and non-convex domains in both two and three dimensions demonstrate the robustness and efficiency of the proposed adaptive methodology.

**Analysis and Numerical Simulations for Coupled Flow-Temperature Models**
Ziehm, Antonia; Hergl, Chiara; Lankeit, Johannes; Wick, Thomas
*Leibniz University Hanover, Germany*
15:00

Numerous current areas of research use thermally driven fluid flow exposed to laser heating. These include 3D laser printing for component construction, waveguide writing and medical applications of laser therapies. However, mapping the physical processes involved is a very complex task due to the fluid's interaction with the heat generated by the laser. Consequently, even comparatively simple configurations are far from trivial to model and require careful mathematical and numerical analysis. In order to analyse the dynamics of such systems, we examine a thermally driven fluid flow subjected to laser heating using the example of water in a cube that is heated with a pair of lasers. Consequently, the Navier–Stokes equations are coupled with the heat equation. Due to the strong coupling of density and viscosity with temperature, the resulting system of partial differential equations is highly nonlinear, reflecting the physical interplay between buoyancy effects, viscous dissipation and thermal diffusion. We prove the existence of a global weak solution and the uniqueness of a local-in-time strong solution. These analytical results provide a rigorous foundation for subsequent numerical investigations. A finite-element implementation using deal.II enables the full model to be simulated numerically. Material parameters cannot be defined for realistic materials without variation. To solve this complex problem with limited computational effort, we use Proper Orthogonal Decomposition (POD) as a model order reduction technique. This significantly reduces the computational cost while retaining the essential dynamical behaviour of the full system.

**Gradient-robust flow modeling in the context of energy transfer**
Neutsch, Constanze; Wollner, Winnifried
*Universität Hamburg, Germany*
15:20

Gradient-robust flow modeling in the context of mixed finite elements is a valuable approach for ensuring
the invariance of the velocity with respect to gradient forces. A suitable modification of the discrete problem, proposed by Linke et al., cures the missing $L_2$-orthogonality by mapping discretely divergence-
free functions to divergence-free ones by utilizing H(div)-conforming finite element spaces. The applicability of this gradient-robust flow modeling was also shown in the context of PDE-constrained optimization by considering stationary incompressible Stokes equation (see work of Merdon and Wollner). In this talk we discuss the extension of these results to control problems constrained by a stationary incompressible Navier-Stokes equation.

**Finite element error estimates for the approximate computation of normal derivatives**
Löscher, Richard; Steinbach, Olaf
*TU Graz, Austria*
15:40

After computing the finite element solution of some boundary value problem with Dirichlet boundary conditions we are interested in the direct computation of the normal derivative, which is of interest in many applications. We will present related error estimates in the natural Sobolev trace space which is $H^{-1/2}(\Gamma)$. Numerical results confirm the theoretical findings.

## S18.05: Model order reduction, splitting, solution schemes

Date: March 18, 2026 16:30–18:30
Room: KI, M11.71
Chair(s): Bertrand, Fleurianne

**A-priori error analysis for space-time POD for a linear parabolic problem**

Gräßle, Carmen (1); Heiland, Jan (2); Marquardt, Jannis (1)

*1: Technische Universität Braunschweig, Germany*
*2: Technische Universität Ilmenau, Germany / Max-Planck-Institut für Dynamik komplexer technischer Systeme Magdeburg, Germany*

16:30

In this talk, we consider a linear parabolic evolution problem and apply space-time proper orthogonal decomposition (POD) (M. Baumann, P. Benner, J. Heiland: Space-time Galerkin POD with application in optimal control of semilinear partial differential equations, SIAM J. Sci. Comput. 40(3), 2018). Our main result is an a-priori error estimate that quantifies the difference between the original full order solution and the reduced order approximation obtained by space-time POD. Starting from the classical splitting of the total error into the POD projection error and the reduced model error, the dependence on spatial and temporal variables gives rise to new challenges in the proof. We present the resulting bound and discuss practical aspects. Numerical examples illustrate our findings.

**Model order reduction of wave propagation in the con text of damage identification**

Burmester, Hannah; Gräßle, Carmen

*TU Braunschweig, Germany*

16:50

Parameter dependent partial differential equations (PPDE) are used to model various real-world phenomena. In the process of solving the PPDE numerically, high-dimensional systems of equations arise which often lead to high computational efforts for example in multi query scenarios. This motivates the use of model order reduction techniques. The basic procedure in model order reduction is to replace a high-dimensional model with a model of reduced dimension without too much loss in accuracy. A classic wave equation is considered to model wave propagation in damaged material. The damage is modelled as a local reduction in the wave propagation velocity; causing the reflection of a propagating wave at the damage. The wave equation is discretized in space and time using finite elements and the Crank-Nicoloson method, respectively. For the model order reduction of the resulting high-dimensional model, a reduced basis method with a POD-Greedy approach is implemented. Model order reduction is difficult for a hyperbolic equation like the considered wave equation. Moreover, the success of the model order reduction highly depends on choosing a suitable parameter set during the reduction process. While a larger parameter set leads to more insight on the behaviour of the high order model, it also prolongs the reduction process. Therefore, strategies are investigated to simplify the model order reduction process with suitable parameter choices.

**A bulk-surface splitting scheme for the semi-linear wave equation with kinetic boundary conditions**

Altmann, Robert; Morandin, Riccardo

*OvGU Magdeburg, Germany*

17:10

In this talk we consider wave equations with dynamic boundary conditions. Unlike more commonly used boundary conditions like Dirichlet or Neumann, these ones do not neglect the effects of the momentum of the wave on the boundary. More specifically, we study a system where the wave equation on the bulk is coupled to a wave equation on the surface. Splitting the bulk and surface variables leads to a natural interpretation of the system as a partial differential-algebraic equation (PDAE).
We exploit this formulation to develop numerical discretization schemes. First, a spatial discretization using bulk-surface finite elements leads to a finite-dimensional differential-algebraic equation (DAE). Then, by approximating the algebraic constraint by using delay terms, we obtain a delay differential-algebraic equation (DDAE) where the bulk and surface dynamics are decoupled. This finally allows us to implement a temporal discretization method, which alternates steps in the bulk and in the surface of the system. We demostrate the qualities of the scheme with both a convergence analysis and numerical results.

**A discrete gradient scheme for preserving QSR-dissipativity**
Karsai, Attila; Schulze, Philipp
*Institute of Mathematics, Technische Universität Berlin, Berlin, Germany*
17:30

Jan Willems formalized processes that cannot generate energy internally by introducing the concept of dissipative dynamical systems. For these systems, changes in energy can only occur due to an external energy supply or dissipation effects. Unfortunately, dissipative properties tend to deteriorate in numerical computations, especially in nonlinear systems. Discrete gradient methods can help mitigate this problem. In this talk, we present a structure-preserving time discretization scheme based on discrete gradients for systems that are dissipative with a quadratic supply rate.

**On Convolution Quadrature based Variational Integrators of Fractional Dynamics**
Hariz, Khaled (1); Ober-Blöbaum, Sina (1); Jiménez, Fernando (2)
*1: Paderborn University, Germany*
*2: Technical University of Madrid*
17:50

Some physical phenomena, as in anomalous damping and deformations, may not be accurately captured by classical models. The fractional calculus plays an important role in describing such phenomena. The main reason why fractional differential equations (FDEs) are being used to model real phenomena is that they are nonlocal in nature, that is, a realistic model of a physical phenomenon depends not only on the actual time but also on the previous one. The analytic solutions of FDEs are however not always available. Dealing with dynamical systems subject to fractional damping, a novel approach was proposed in "F. Jiménez and S. Ober-Blöbaum Fractional Damping Through Restricted Calculus of Variations, JNS (2021)" to formulate it in a purely variational way. We derive higher-order fractional variational integrators for this approach using Rung-Kutta convolution quadratures (RKCQs) and some numerical tests are provided. We are specially interested in the CQ based on Lobatto IIIC. Preservation properties such as energy decay as well as convergence properties are investigated numerically and proved for 2nd order schemes. The presented schemes reach 2nd, 4th and 6th accuracy order.

**Shooting Methods for Boundary Value Problems of Fractional Differential Equations**
Pulch, Roland; Singh, Abhishek Kumar
*Universität Greifswald, Germany*
18:10

We consider two-point boundary value problems of fractional differential equations (FDEs) including a Caputo derivative with a fractional order in the range (0,1) or (1,2). The numerical solution of a boundary value problem is investigated using shooting methods or similar techniques. Consequently, initial value problems of FDEs are integrated to determine the final numerical solution. The generated nonlinear systems of algebraic equations can be solved by methods of Newton-type. However, these methods often fail if the problem is sensitive and the initial guess is not sufficiently close to the true solution. Alternatively, a defect can be reduced nearly to zero using minimisation schemes. For example, differential evolution represents a stochastic population-based optimisation method, that can be used for such a task. Furthermore, we examine the application of sensitivity matrices, which include the partial derivatives of the solution with respect to the initial values, in the shooting methods. The sensitivity matrices can be computed simultaneously in the numerical integration of the initial value problems. We present results of numerical computations for test examples of FDEs.

**S18.06: Applications of PDEs**
Date: March 19, 2026 08:30–10:30
Room: KI, M11.71
Chair(s): Frei, Stefan

**Semi-explicit Time Discretization of Thermo-poroelasticity**

Altmann, Robert (1); Maier, Roland (2); Schmeck, Jochewed (1) 08:30
*1: Otto-von-Guericke-Universität Magdeburg, Germany*
*2: Karlsruhe Institute of Technology, Germany*

We present a decoupling approach for solving the equations of thermo-poroelasticity, which describe the behavior of an elastic solid medium containing fluid-filled pores. The model is a coupled system consisting of one elliptic equation and two parabolic equations. To solve this system, one must determine the elastic displacement (mechanics), the fluid pressure (flow), and the temperature. In this talk, we focus on the time discretization of such systems. In particular, we introduce a semi-explicit scheme that fully decouples the equations. The main idea is to identify the scheme as an fully implicit discretization of a corresponding delay equation
of parabolic type. The convergence analysis provides sufficient conditions on the physical parameters that guarantee first-order convergence of the method.

**A locking-free and loosely coupled Robin-Robin scheme for the incompressible fluid-poroelasticity interaction.**

Yue, Xiaohe (1,2); He, Wenlong (3); Wick, Thomas (2); Zhang, Jiwei (3); Zheng, Haibiao (2) 08:50
*1: Leibniz University Hannover, Germany*
*2: East China Normal University, China*
*3: Wuhan University,China*

We propose a fully parallelizable and loosely coupled scheme for the incompressible fluid-fully dynamic poroelasticity interaction (FPSI) problem, which is locking-free for extreme model parameters. By introducing two new auxiliary variables, the poroelasticity system is reformulated into a four-field formulation, which can be regarded as a coupling of a Stokes-like system and a diffusion system. The decoupled scheme is constructed based on Robin-Robin type coupling conditions, evaluating the right-hand side of the these conditions at the previous time step. The resulting scheme is fully parallel, meaning that the fluid subsystem and poroelasticity subsystem can be solved independently at each time step without expensive sub-iterations. Furthermore, we prove that the scheme is unconditionally stable and provide an error estimate showing that the convergence in the $H^1$ norm is optimal. The error analysis demonstrates that our scheme is robust against extreme model parameters, thereby eliminating the locking inherent in poroelasticity system. Various numerical experiments are presented to validate the stability, convergence and locking-free performance of the proposed scheme.

**Numerical approximation of the the dynamic poroelasticity equation in first order form**

Shamko, Pavel; Bause, Markus 09:10
*Helmut Schmidt University, Germany*

We study the numerical approximation of the Biot poroelasticity equations, which describe the coupled interaction between elastic deformation of a porous solid and fluid flow in the pore space. In their classical second-order formulation, the model consists of a momentum balance for the solid displacement and a mass balance for the pore pressure. The system couples linear elasticity with Darcy flow through the Biot coefficient and a storage term.

To enable a unified space-time discretization and to expose the underlying operator structure of the coupled problem, we reformulate the Biot system by introducing the auxiliary variables
$v = \partial_t u$ for the solid velocity,
$\sigma = C\varepsilon(u)$ for the stress tensor,
and $q = -K\nabla p + \alpha v$ for the fluid flux,
the governing equations can then be written as an Evolutionary equation
$(\partial_t M_0 + M_1 + A)U = F$.
This formulation yields a block-structured system that is first order in both time and space and naturally incorporates inertia, elasticity, and fluid flow effects.

The resulting problem is discretized using a space-time finite element method with discontinuous Galerkin discretization in time. On each time interval, this approach leads to a fully coupled algebraic system that simultaneously resolves all unknowns and weakly enforces temporal continuity by means of jump terms. We derive the algebraic system arising from the space-time discretization and briefly discuss its structural properties.

To efficiently solve the resulting linear systems, we employ a GMRES iteration preconditioned by a geometric multigrid method. The multigrid preconditioner is tailored to the block structure of the first-order formulation and is applied to the spatial discretization, aiming at robustness with respect to mesh refinement and material parameters.

Finally, we present numerical benchmarks that confirm the expected convergence rates of the space-time discretization. In addition, we investigate the convergence behavior of selected goal quantities of interest and analyze the solver performance by reporting the number of GMRES iterations required per time step. The numerical results demonstrate the accuracy, robustness, and computational efficiency of the proposed space-time discretization and solver strategy for poroelasticity problems.

**Thermobaricity-driven circulation and water renewal in deep, low-salinity lakes**

Irmscher, Jonathan; Richter, Thomas
*Otto-von-Guericke-University, Germany*

09:30

Stratification strongly influences lake circulation, oxygenation, and biogeochemical exchange. In stably stratified lakes, deep and surface waters can differ markedly in chemical composition. Changes in mixing intensity or overturn events can therefore alter oxygen levels and water quality by redistributing reduced or nutrient-rich deep water.

Accurate modelling of circulation and air-water oxygen exchange in deep, low-salinity lakes requires thermobaric effects, i.e. the pressure-temperature dependence of water density. In such systems, density differences at depth can be small enough that thermobaricity becomes a primary driver of vertical exchange and renewal.

We investigate thermobaricity-driven circulation in a simplified setting using a 2D Boussinesq Navier-Stokes framework in which the buoyancy term is derived from a water equation of state. To assess renewal and stratification persistence, we introduce a passive “water age” tracer. We first compute a time-periodic solution for the flow and temperature fields, and then transport the age tracer over many cycles using this periodic state. This approach enables efficient long-term estimates of water renewal time scales and their sensitivity to thermobaric forcing, providing a simplified assessment of physical stability in deep-lake stratification.

**A Temporal Multiscale Approach to Tidal Forcing in Ice-Sheet Dynamics**

Reddig, Celine; Richter, Thomas
*Otto von Guericke University, Germany*

09:50

In general, ice sheets and glaciers can be modelled as very slow, viscous fluids, which allows for large time steps on the order of years. However, over the past few decades, observations and theoretical studies have shown that ice streams exhibit significant, short-term responses when it comes to external forcing due to ocean tides, which induce non-linear variations in the ice velocity.
Short-term models typically incorporate viscous-elastic ice rheologies to capture these effects. However, resolving the associated dynamics requires very small time steps on the order of minutes, making long-term simulations computationally challenging.
To address this, we propose a temporal averaging approach that incorporates short-term tidal effects into efficient, long-term simulations. We present first results based on a two-component modelling framework. The long-term component models the ice sheet as a viscous fluid governed by the p-Stokes equations with free surfaces. The short-term component describes the elastic response of the ice to tidal forcing, modelled by an elasticity problem driven by variations in hydro-static pressure due to ocean tides. This leads to a variational inequality of Signorini type, reflecting intermittent contact between the ice and the bedrock.

As the tidal cycle causes the ice–bedrock contact zone to evolve in time, the basal friction varies accordingly. By exploiting the periodic nature of the tidal forcing, we derive averaged friction coefficients that can be incorporated into the basal friction law of the viscous, long-term ice-flow model. The averaged friction coefficients are updated after a time step in the long-term model to take the geometric deformation of the ice sheet into account.
This approach enables efficient simulations that retain the essential influence of short-term tidal dynamics on ice-stream motion, and relies on a clear separation between the short tidal time scale and the long-term viscous evolution of the ice sheet.

**Self-propulsion of an immersed body via rotation and deformation**
Edelmann, Joris; Richter, Thomas
*Otto von Guericke University Magdeburg, Germany*
10:10

A body immersed in a fluid (swimmer) can move by shifting its center of mass and through deformation. We assume that both actions are periodic and that the resulting force acting on the body is mean-free. Considering mass shift only, we used a 3-dimensional simulation, in which the body can translate and rotate. This is an extension to previous work, where we assumed cylindrical symmetry [1]. External forces are assumed to act at arbitrary points, introducing rotational dynamics into the system, leading to the emergence of new phenomena in contrast to [1].
We present the numerical modeling of this problem using an ALE formulation of the fluid-solid interaction, with enhanced techniques to improve convergence to periodic limit cycles.
Furthermore, we show the initial results of the impact of body deformation on motion dynamics.
This work is conducted in collaboration with M.M. Karakouzian, G.P. Galdi, and T. Richter.
[1] J. Edelmann, G. P. Galdi, M. M. Karakouzian, and T. Richter, On the propulsion of a rigid body in a viscous liquid by time-periodic force with
a zero average, arXiv (2025)

## S18.07: Discretization of PDEs
Date: March 19, 2026 14:00–16:00
Room: KI, M11.71
Chair(s): Haubold, Tim

**Efficient discontinuous Galerkin methods leveraging local–global structures**
Lederer, Philip L. (1); Lehrenfeld, Christoph (2); Stocker, Paul (3); Voulis, Igor (2)
*1: University of Hamburg, Germany*
*2: University of Göttingen, Germany*
*3: University of Vienna, Austria*
14:00

Discontinuous Galerkin (DG) methods provide great flexibility for solving partial differential equations numerically, but this often comes at the cost of a large number of unknowns. In this talk, we present Embedded Trefftz–DG methods, which dramatically reduce unknowns by embedding an element-wise discrete space that lies in the kernel of the PDE operator, either exactly or approximately. The solution is split into a local part, conforming to the PDE, and a global part, which enforces inter-element continuity and boundary conditions via standard DG formulations. This is set within a framework that enables a rigorous a priori error analysis and applies to a wide range of PDEs. We present examples ranging from wave propagation to fluid flow, and demonstrate the method's robustness on challenging discretizations, such as highly anisotropic meshes. The talk will highlight both the underlying theoretical principles and representative numerical results, showing that Embedded Trefftz-DG methods retain optimal convergence rates while achieving substantial reductions in computational cost.

**Tangential Crouzeix Raviart Finite Elements for the Surface Stokes Equation**

Chowdhury, Manisha (1); Mehlmann, Carolin (1); von Wahl, Henry (2) 14:40

*1: Institute of Analysis and Numerics, Otto-von-Guericke University Magdeburg, Germany*
*2: Institute for Mathematics, Friedrich Schiller University Jena, Germany*

Recently, increasing attention has been paid to finite element discretizations of vector-valued flow problems posed on curved surfaces. In this work, we study a surface Stokes system defined on a two-dimensional manifold embedded in three-dimensional space. The surface velocity field is approximated using a nonconforming Crouzeix–Raviart finite element on a polyhedral approximation of the surface, while the pressure is discretized by piecewise constant functions. The governing equations involve the symmetric strain-rate tensor, whose approximation with Crouzeix–Raviart finite elements leads to spurious oscillations in the velocity field due to the presence of a non-trivial kernel. To address this issue, we derive a stabilized formulation of the momentum equation. Further, we show that this finite element pair satisfies the inf–sup condition and derive optimal a priori error estimates in both the energy-norm and the L2-norm. These theoretical results are corroborated by numerical experiments.

**On the numerical treatment of the stochastic Cahn-Hilliard equation with double-obstacle potential**

Banas, Lubomir (2); Metzger, Stefan (1) 15:00

*1: Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*
*2: Bielefeld University, Germany*

The Cahn-Hilliard equation is a deterministic model for the description of phase separation processes in metal alloys, which occur if the alloy is rapidly cooled below a critical temperature. This equation can be interpreted as a gradient flow of the Ginzburg-Landau energy functional, which consists of a gradient term and double-well potential favoring phase separation. If the quench is shallow, i.e. the temperature is still close to the critical temperature, the double-well potential can be approximated by a smooth fourth-order polynomial. Yet, in the deep quench limit, i.e. when the temperature is significantly smaller than the critical temperature, a singular double-obstacle potential is the better choice. It is also well-known that in particular the early stages of the separation process are heavily influenced by thermal fluctuations which are not included in the deterministic description.
In this talk, we discuss the numerical treatment of the stochastic Cahn-Hilliard equation with double-obstacle potential and conservative noise on a periodic domain.
In particular, we propose a fully discrete finite element scheme and present a convergence result. Conceptually, our proof relies on monotonicity arguments and omits the application of Skorokhod's theorem, which allows us to show convergence towards probabilistically strong solutions. We conclude by presenting numerical simulations underlining the practicality of the proposed scheme and the importance of the additional stochastic fluxes.

**Generalized shape operator for nonlinear shells**

Neunteufel, Michael (1); Gopalakrishnan, Jay (2); Schöberl, Joachim (1) 15:20

*1: TU Wien, Austria*
*2: Portland State University, USA*

In computing the bending energy of nonlinear shells, the surface curvature represented by the shape operator plays a fundamental role. Discrete differential geometry (DDG) aims to approximate curvature quantities of discretized domains. By embedding DDG within a finite element context, rigorous numerical analysis tools become available for investigating and extending those algorithms. So-called distributional finite elements are essential in the process. They entail weak regularity, so that differential operators must be understood in the sense of distributions.
In this talk, we approximate the shape operator on surfaces, where the discretized surface is described by Lagrange finite elements, by combining the concept of dihedral angles from DDG with Hellan-Herrmann-Johnson finite elements. Then, we discuss their application to nonlinear Kirchhoff-Love shells by approximating the bending energy term, the difference between the curvatures of the

initial and deformed configurations. We present numerical examples using the finite element library NGSolve (www.ngsolve.org).

**hp-Finite Elements for Elastoplasticity**
Bammer, Patrick (1); Banz, Lothar (2); Schröder, Andreas (2) 15:40
*1: University of Bern, Switzerland*
*2: University of Salzburg, Austria*

We consider a model problem of *elastoplasticity with linearly kinematic hardening*, whose well-established weak formulation is given by a variational inequality of the second kind. This formulation, however, contains a non-differentiable term leading to difficulties in the numerical analysis and computation of a discrete solution. We therefore introduce a mixed variational formulation in which the non-differentiable term is resolved by a Lagrange multiplier. This mixed problem turns out to be equivalent to the variational inequality. The use of biorthogonal basis functions in the discretization with higher-order finite elements allows us to decouple the constraints associated with the discrete Lagrange multiplier. Therefore, the discrete formulation can be rewritten as a system of decoupled nonlinear equations which enables the application of an efficient semismooth Newton solver. We present a priori and a posteriori error estimates for the discrete formulation, and numerical examples that finally confirm the theoretical convergence rates and demonstrate the solver's efficiency.

## S18.08: Applications II of PDEs
Date: March 19, 2026 17:30–18:30
Room: KI, M11.71
Chair(s): Kanschat, Guido

**Modeling Nonlinear Acoustic Wave Propagation with Third-Order Elastic Constants Using the Finite Element Method**
Hölscher, Jonas; Claes, Leander; Förstner, Jens; Henning, Bernd 17:30
*Paderborn University, Germany*

Due to the widespread application of specialized piezoelectric actuators in various applications, accurate simulations have become key components of modern design processes.
Although simulation tools for piezoelectric devices are widely available, nonlinear effects, which occur when exciting near resonance at elevated amplitudes, are often neglected or linearized.
At those resonance peaks the piezoelectric systems exhibit characteristics of highly dynamical nonlinear systems, showing typical nonlinear effects such as frequency shifts, jump phenomena and bifurcations.
To correctly reproduce this behavior, suitable material models must be identified and incorporated into the simulation environment.
Therefore, in this work we present a finite element formulation for nonlinear piezoelectric systems that exhibit a quadratic elastic nonlinearity for the strain-stress relation in the mechanical field. This results in a third-order mechanical material tensor, which can be described using third-order elastic constants. For the electrical field and the piezoelectric coupling linear behavior is assumed. For the model an axisymmetric piezoelectric ring is used, and the simulation is performed in time-domain with harmonic excitation.
Existing methods for incorporating such quadratic nonlinearities simplify or linearize the nonlinear stiffness matrix, since the classical approach of the variational formulation is not suitable. To enable the use of the full set of nonlinear material parameters, the finite element formulation must be derived using tensor notation. This results in tensor-valued element-matrices as well as a tensor-valued nonlinear stiffness matrix, which is unrolled for the simulation process in this work.
Simulation results are presented which show higher order harmonics for the mechanical field in the response spectrum.
This approach can be applied to even higher-order nonlinearities, however, the presented numerical examples focus on quadratic elastic properties.

**Robust Interface-Based Modeling for Nutrient Transport in Porous Media**

boudrari, fadoua 17:50
*Mohammed VI Polytechnic University (UM6P), Morocco*

In agriculture, traditional soil fertilizers are often inefficient due to a mismatch between the timescale of nutrient transport in soil and the timescale of plant uptake, leading to significant nutrient losses and environmental harm. Coated or controlled-release fertilizers aim to reduce these losses by delaying nutrient release into the surrounding soil.

Modeling such systems requires reliable numerical simulation of coupled transport processes in porous media, where diffusion, flow-driven transport, and heterogeneity interact across multiple scales, posing significant challenges for numerical stability and reproducibility.
From a numerical modeling perspective, we show that nutrient release can not be treated as a volumetric soil source, but must instead be modeled as a localized exchange process at the fertilizer–soil interface.

This modeling choice has direct implications for numerical stability and mass conservation. Based on this observation, we derive a mechanistic interface exchange law to represent the release process at the granule boundary. This law is incorporated into a coupled system of transport equations posed in the surrounding porous medium, describing nutrient migration from the granule interface into the soil.

The resulting model describes nutrient transport through diffusion and advection, leading to an advection–diffusion reaction formulation with interface exchange terms.

The coupled system is formulated in a variational setting, which provides a consistent framework for analyzing stability and mass conservation and for discretization using finite element methods. Within this framework, we analyze well-posedness and investigate stability with respect to variations in model parameters and discretization choices.
We examine how geometric resolution and discretization choices influence stability and mass conservation. Interface-resolved meshes are employed to represent interface exchange terms consistently at the discrete level.
The finite element discretization is chosen to ensure stability for advection–diffusion transport and to preserve mass across relevant parameter regimes.
A non-dimensionalization of the governing equations is used to support parameter-dependent analysis. This allows us to identify transport regimes and to study transitions between release dominated and transport-dominated behavior. The analysis remains directly connected to agriculturally motivated case studies.

**A Robust High-Order Computational Technique for Space-Time Fractional Stochastic Nonlinear Diffusion-Wave Equations**

Singh, Dr Anant Pratap (1); Singh, Dr Vineet Kumar (3); Maurya, Dr Rahul (2) 18:10
*1: J K Lakshmipat University, India*
*2: IIT (BHU) Varanasi*
*3: IIT (BHU) Varanasi*

In this study, a novel numerical approach is proposed and analyzed for solving space–time fractional stochastic nonlinear diffusion-wave equations. The method employs an implicit scheme, constructed by integrating a matrix transformation technique to discretize the Riesz fractional derivative in space, alongside a $(3-\alpha)$-order approximation for the Caputo fractional derivative in time. To address the nonlinear source term, a Taylor series expansion is applied for linearization, enabling efficient computation of solutions for this class of fractional models. The scheme is shown to achieve convergence of order $\beta$ in the spatial domain and $(3-\alpha)$ in the temporal domain. A rigorous theoretical analysis confirms the unconditional stability of the method and provides optimal error estimates in both space and time. Additionally, a series of numerical experiments validate the accuracy, consistency,

and computational efficiency of the proposed algorithm, demonstrating its ease of implementation and reduced computational cost.

## S18.09: Numerical solution schemes: GMG, DD, FFT, HPC

Date: March 20, 2026 08:30–10:30
Room: KI, M11.71
Chair(s): Wick, Thomas

### On geometric multigrid convergence and its application to space-time FEM

Bause, Markus (1); Margenberg, Nils (2)
*1: Helmut Schmidt University, Germany*
*2: Otto von Guericke University Magdeburg, Germany*
08:30

Space-time finite element methods (STFEMs) have demonstrated their potential for the accurate and efficient approximation of incompressibe viscous flow and related problems on computationally feasible grids. STFEMs lead to high dimensional algebraic systems of equations. Their fast solution by robust iterative solvers, in particular if three space variables are involved, continues to remain a challenging problems. Algebraic Multigrid (AMG) and geometric multigrid (GMG) methods have been applied for the solution of (linearized) STFEM algebraic systems, either in holistic or time marching form. Also, multigrid methods have been used as preconditioners for Krylov subspace iterations, like GMRES, to enhance their robustness [M. Anselmann, M. Bause, A geometric multigrid method for space-time finite element discretizations of the Navier–Stokes equations and its application to 3d flow simulation, ACM Trans. Math. Softw., 49 (2023), Article No.: 5]. In the context of nonstationary problems, the convergence of GMG has been studied rarely in the literature so far [M.J. Gander, M. Neumüller M, Analysis of a new space-time parallel multigrid algorithm for parabolic problems, SIAM J. Sci. Comput., 38 (2016), A2173-A2208].

Here, we present an analytical proof of convergence for the two grid convergence of the GMG method applied to STFEM methods for the prototype problem of the heat equation. The analysis provides insights into the GMG mechanisms and parameter dependencies. The framework is sufficient flexible to be generalized to more complex systems, like incompressible viscous flow. Further, we discuss geometric GMG preconditioning in a more general framework, including hp multigrid techniques with coarse grid correction in the space and time polynomial orders and for the spatial mesh [N. Margenberg, M. Bause, P. Munch, An hp multigrid approach for tensor-product space-time finite element discretizations of the Stokes equations, SIAM J. Sci. Comput., 47 (2025), pp. 1503-1529].

### Krylov-Based Iterative Methods for Linear Port-Hamiltonian Systems

Maier, Stefan; Marheineke, Nicole
*Trier University, Germany*
08:50

This talk addresses efficient structure-preserving numerical integration for linear closed port-Hamiltonian systems based on iterative techniques. This class of systems is characterized by a quadratic Hamiltonian representing the energy of the system and exhibits dissipative behavior, with solutions satisfying a dissipation inequality. A special case arises in the absence of dissipation, in which the system is energy-conserving.
To preserve the energy behavior at the discrete level, Gauss collocation methods are particularly well suited. They can be reformulated in terms of diagonal Padé approximations. This reformulation allows the numerical solution to be expressed as the action of a matrix-valued diagonal Padé approximation on a vector. The Padé approximation can be represented by either numerator and denominator polynomials or by its partial fraction decomposition, both of which require the solving of linear systems.
For large sparse matrices, Krylov-type subspace methods provide an efficient framework for computing the matrix-function actions. Both minimal residual and Galerkin conditions can be employed. We present several approaches based on polynomial and partial fraction representations and discuss their structure-preserving properties, convergence behavior, and computational efficiency.

**An FFT-based solver for heterogeneous micromagnetics**

Lendvai, Jonas (1); Vorwerk, Maximilian (1); Schneider, Matti (1,2,3); Schröder, Jörg (1) 09:10
*1: University of Duisburg-Essen, Essen, Germany*
*2: Center for Nanointegration Duisburg-Essen (CENIDE)*
*3: Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany*

Micromagnetism describes the evolution of the magnetization field under the combined action of magnetostatic interactions, magnetic exchange fluxes, and magnetic anisotropy. Because these mechanisms act across multiple spatial and temporal scales, reliable simulations require dedicated numerical techniques capable of resolving both local grain-level behavior and long-range interactions. In the talk at hand, we present an implicit FFT-based solver for the Landau-Lifshitz-Gilbert (LLG) equation tailored to polycrystalline ferromagnets with insulated grain interfaces. We investigate its numerical behavior across a set of representative computational examples.

**Numerical approximation of partial differential equations using periodic extensions and high-performance computing**

Doghman, Jad; Amlani, Faisal 09:30
*Ecole Normale Supérieure Paris-Saclay, France*

Numerically solving partial differential equations (PDEs) plays a key role in various scientific fields such as structural and fluid mechanics, as closed-form analytical solutions are rarely obtainable. Considerable effort has been devoted to developing robust and efficient numerical methods for solving a wide spectrum of PDEs. Some of these approaches remain computationally prohibitive for stiff regimes, while others suffer from severe time-step restrictions or excessive numerical dissipation, leading to large errors relative to the exact solutions (e.g., reaction-diffusion with very fast reaction). To address these limitations, we employ the Fourier Continuation (FC) method, a framework based on SVD and Gram polynomials that extends the FFT-based Fourier spectral approach to non-periodic domains and suppresses the Gibbs phenomenon that typically occurs at the domain boundaries, provided that the underlying function is smooth inside the physical domain. FC generates a regular periodic extension by appending a short auxiliary piece of domain (e.g., a segment in 1D) in which the originally non-periodic function is blended to zero via a low-degree polynomial from both extremities. The interpolation of the two resulting blendings produces a smooth continuation over the slightly extended domain. Leveraging the substantial speedup and spectral accuracy that FC offers over finite element and finite difference methods, we have developed a dedicated C++ solver within a high-performance computing (HPC) framework to highlight its solving efficiency and competitiveness. Several other periodic-extension techniques with goals similar to FC have been established in the literature, most notably barycentric rational interpolation and a range of extrapolation/blending methods for constructing smooth periodic continuations. These alternative approaches have different properties and characteristics, and are implemented in the same high-performance solver, enabling a consistent and fair comparison with FC on a benchmark wave equation in terms of speed, accuracy, and memory consumption. The present C++ solver is cross-platform, self-sufficient and does not rely on external linear algebra libraries (e.g., Eigen or Armadillo). It has been specifically tailored for the FC method and is being extended to tackle challenging continuum mechanics problems, including micropolar hyperelasticity and phase-field models.

**Multilevel Schwarz Methods for the Coupled Stokes–Darcy Problem**

Zhang, Haicheng (1,2); Kanschat, Guido (1) 09:50
*1: Heidelberg University, Germany*
*2: East China Normal University, China*

We present a monolithic multigrid solver for a strongly mass-conservative mixed finite element discretization of the coupled Darcy-Stokes problem. An overlapping Schwarz smoother is employed and different treatments of boundary degrees of freedom are compared. In particular, we investigate the effect of velocity and pressure boundary conditions in the Darcy subdomain, as well as the inclusion of boundary unknowns in the vertex patches. Numerical results show that the convergence behavior,

especially for the pressure, strongly depends on the smoother design. With a consistent treatment of boundary degrees of freedom, the proposed method is robust and requires less than 10 iterations for high-order discretizations.

**Performance of vertex-patch smoothers on GPU architectures**

Kanschat, Guido; Cui, Cu
*Universität Heidelberg, Germany*

10:10

We discuss the numerical performance of vertex-patch smoothers and their implementation on GPUs. In particular, we investigate efficient local solvers based on fast diagonalization in the context of Poisson, Stokes, and biharmonic equations. In the implementation, particular aspects of memory management make or break performance. In computational experiments, we show that we can get a high utilization of the computing power of an A100 GPU.

## S19: Optimization of differential equations

Organizer(s): Azmi, Behzad *(University of Konstantz)*
Schaller, Manuel *(Technische Universität Chemnitz)*

## S19.01: Optimal control and stabilization of evolution equations

Date: March 17, 2026 08:30–10:30
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

### LQ optimal control for infinite-dimensional passive systems

Hastir, Anthony; Jacob, Birgit
*Bergische Universität Wuppertal, Germany*
08:30

We study the Linear-Quadratic optimal control problem for a general class of infinite-dimensional passive systems, allowing for unbounded input and output operators. We show that under mild assumptions, the finite cost condition is always satisfied. Moreover, we give an explicit bound on the norm of the optimal cost operator. In the case where the system is energy preserving, the unique optimal control is given together with the corresponding optimal cost operator. In this case, we derive an explicit solution to an adapted operator Riccati equation. We apply our results to boundary control systems and first-order port-Hamiltonian systems.

### The dissipation inequality for infinite-dimensional systems

Reis, Timo
*Technische Universitaet Ilmenau, Germany*
08:50

This talk addresses the dissipativity of linear infinite-dimensional systems with respect to quadratic supply rates. We present an operator inequality that characterizes dissipativity and provides an explicit expression for the dissipation rate. Connections to linear–quadratic optimal control problems on the nonnegative real half-line will also be discussed.

### Optimal control of a nonlinear kinetic Fokker-Planck equation

Breiten, Tobias (1); Kunisch, Karl (2)
*1: TU Berlin, Germany*
*2: University of Graz & RICAM Linz, Austria*
09:10

An optimal tracking control problem is studied for a nonlinear, nonlocal kinetic Fokker–Planck equation modeling mean-field interactions with distance-dependent noise. Since the equation is only hypocoercive and the control operator unbounded in the canonical state space, classical variational techniques are not directly applicable. The concept of admissible control operators is therefore employed. Local Lipschitz estimates for the nonlinearities are derived and incorporated into a fixed-point argument to establish local well-posedness. Due to hypocoercivity, standard compactness arguments fail to ensure the existence of optimal controls, requiring alternative analytical methods.

**Domain-uniform bounds in optimal control: Exponential decay of perturbations and efficient domain decomposition preconditioning**

Oppeneiger, Benedikt (1,2); Egger, Herbert (3,4); Göttlich, Simone (5); Schaller, Manuel (2); Takacs, Stefan (3); Worthmann, Karl (1)

*1: Technische Universität Ilmenau, Germany*
*2: Technische Universität Chemnitz, Germany*
*3: Johannes-Kepler-Universität Linz, Austria*
*4: Johann Radon Institute for Computational and Applied Mathematics of the Austrian Academy of Sciences Linz, Austria*
*5: University of Mannheim, School of Business Informatics and Mathematics*

09:30

We consider linear-quadratic optimal control problems constrained by general evolution equations. We analyze the corresponding necessary first-order optimality conditions which form an infinite-dimensional linear equations system. Based on domain-uniform stabilizability and detectability conditions, we establish existence, uniqueness, and stability of solutions. In particular we derive upper and lower bounds on the linear operator appearing in the first order optimality system.

These estimates can be leveraged in order to obtain two main results:

First we are able to show that the optimally controlled system is robust with respect to spatially localized perturbations in the sense that these perturbations only have an exponentially localized effect on the optimal solution.

Second we are able to use a minimal residual (MINRES) method with domain decomposition preconditiong to efficiently compute a numerical solution of the optimal control problem. We show that the number of iterations until convergence is independent of the number of subdomains. The necessary computations may be easily parallelized. Therefore using our theory and adapting the number of processing units optimal control problems of arbitrary size may be solved without any increase in computing time.

Finally we characterize our notion of domain-uniform stabilizability and detectability for a large class of hyperbolic and elliptic equations.

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[3] B. F. Oppeneiger, H. Egger et al. “Stability and convergence of iterative solvers for a class of elliptic optimal control problems”. In preparation.

**Finite-Dimensional MOR-Based MPC for the 2D Navier-Stokes Equations**

Sauer, Felix (1); Azmi, Behzad (2); Frei, Stefan (2)

*1: Weierstrass Institute for Applied Analysis and Stochastics, Germany*
*2: University of Konstanz, Germany*

09:50

We study the stabilisation of a two-dimensional incompressible fluid flow, described by the velocity field $y(t,x)$ solving the Navier-Stokes equations, towards a prescribed reference flow $\hat{y}(t,x)$ by means of finite-dimensional model predictive control (MPC). The control acts through a finite number of distributed actuators supported in a subregion of the domain. By introducing the translated variable $v = y - \hat{y}$, we reformulate the problem as the stabilisation of the shifted system towards $v \equiv 0$. In the MPC framework, at each sampling time a finite-horizon optimal control problem for the translated system is solved, only the first part of the optimal control is applied, and the optimisation horizon is then shifted forward in time. To reduce the substantial computational cost of repeatedly solving high-dimensional optimal control problems, we incorporate a model-order reduction (MOR) step based on proper orthogonal decomposition (POD). Reduced bases for both state and adjoint variables are constructed from snapshot data and used to define a surrogate optimal control problem on each prediction horizon that can be solved much more efficiently. Numerical experiments for a driven

cavity-type disc geometry and a more challenging channel-flow configuration with vortex shedding are presented. The results illustrate the influence of the prediction horizon, viscosity and actuator layout, and demonstrate that the POD-based MPC significantly reduces runtimes while preserving stabilisation performance.

**A port-Hamiltonian perspective on minimum cost network flow problems**

Landwehr, Lina (1); Doganay, Onur Tanil (2); Klamroth, Kathrin (1); Lang, Bruno (1); Stiglmayr, Michael (1); Totzeck, Claudia (1)

*1: University of Wuppertal, School of Mathematics and Natural Sciences, IMACM, Gaußstraße 20, 42119 Wuppertal, Germany*

*2: TU Berlin, Institute of Mathematics, Straße des 17. Juni 136, 10623 Berlin, Germany*

10:10

This work develops a port-Hamiltonian viewpoint on minimum cost network flow problems and shows how this structure can model both static and time-dependent flows on graphs. Classical minimum cost flow models are usually formulated as linear programs and solved with standard network optimization methods, but extending them to time-varying or nonlinear settings while preserving network structure is challenging or solving them is expensive. Port-Hamiltonian systems offer an energy-based framework that encodes conservation laws and interconnection structure in skew-symmetric matrices, which can be adapted to network flows by combining node variables and edge flows in a single state.

We formulate an optimal control problem for port-Hamiltonian dynamics and derive first-order necessary conditions via an adjoint system, which are then used in gradient-based numerical methods. Static minimum cost flow problems appear as stationary solutions of a suitable port-Hamiltonian system, while dynamic flow problems are treated as optimal control problems with time-dependent costs and regularization of the control. Capacity restrictions are handled using projections and barrier terms, leading to an algorithm that respects flow conservation.

## S19.02: Robustness and uncertainty

Date: March 17, 2026 16:30–18:30
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Optimization and control of differential equations under uncertainty**

Guth, Philipp A.

*RICAM, Austrian Academy of Sciences, Austria*

16:30

Differential equations with random coefficients have become a popular way of incorporating uncertainty into models for engineering or physical processes. One reason behind their success is the ability to integrate knowledge of governing physical equations while accommodating randomness, which may reflect, for instance, missing data, measurement uncertainties, material imperfections, or external influences. In optimization and optimal control problems governed by random differential equations, a careful treatment of uncertainty is indispensable, since even small parameter variations may change the system's characteristics, such as its stability properties.

A common approach is to combine the control objective with a risk measure in order to account for rare but critical events, and to approximate the resulting cost functional by a sample average. This leads to large deterministic optimization problems that can be solved using (stochastic) gradient-based methods, but which often become prohibitively expensive when high accuracy is required. Multilevel strategies offer an effective mitigation by exploiting hierarchies of discretizations to balance sampling and discretization errors, thereby significantly reducing computational cost. Computational efficiency can be further improved when the dependence on uncertain parameters is sufficiently smooth, allowing higher-order cubature methods, such as quasi-Monte Carlo methods, to achieve improved convergence rates independently of the dimension. It will be demonstrated that

this favorable parametric regularity arises in a broad class of control problems governed by differential equations.

In the second part of the talk, the focus is shifted from open-loop optimization to feedback control under uncertainty. The a priori synthesis of feedback laws for sampling and spectral discretizations of the uncertainty is discussed, including recent results on the construction of feedback controllers for risk-averse objectives based on nonlinear risk measures. Finally, a dynamic data-driven setting is considered, in which feedback control is combined with adaptive parameter estimation. In this framework, a computational model evolves alongside the physical system, measurement data are assimilated in real time, and the digital model jointly acts as observer, estimator, and control agent.

**Multilevel Stochastic Gradient Descent for Risk-Averse PDE Constraint Optimization**

Baumgarten, Niklas (1); Guth, Philipp A. (2); Schneiderhan, David (3); Vanzan, Tommaso (4) 17:10

*1: Heidelberg University, Germany*
*2: Johann Radon Institute for Computational and Applied Mathematics, Austria*
*3: Karlsruhe Institute of Technology (KIT), Germany*
*4: Politecnico di Torino, Italy*

We present recent advances of the multilevel stochastic gradient descent algorithm for solving risk-averse PDE-constrained optimization problems. The algorithm uses multilevel Monte Carlo gradient estimation, provides parallel scalability and improved convergence rates, as well as effective control of risk parameters.

In addition, we discuss techniques, such as adaptive batch size and step-size, to further improve performance. Numerical experiments on an elliptic diffusion problem demonstrate the effectiveness and efficiency of the proposed approach.

**Risk averse Kalman filters for systems subject to parametric uncertainties**

Kunisch, Karl (1,2); Schröder, Jesper (2) 17:30

*1: Universität Graz*
*2: RICAM Linz*

The well-known Kalman-Bucy filter yields optimal state reconstructions for linear dynamical systems subject to additive noise in initial state, dynamics, and outputs. It does, however, require exact knowledge of the underlying model and inaccuracies in the system matrix may deteriorate its results.
Taking a deterministic perspective this talk proposes extensions incorporating parametric uncertainties allowing for an explicit treatment of system inaccuracies.
The emphasis lies on risk averse designs reducing the probability of large reconstruction errors. The presentation includes characterizations and analytical properties of the estimators such as regularity results and error bounds. Numerical experiments for two example systems illustrate the theoretical results and investigate the practical impact of risk aversion.

**Towards Robust PDE-Constrained Optimization via Polynimial Chaos Expansion with applications in fiber-spinning**

Witt, Jakob Paulo (1); Blauth, Sebastian (1); Pinnau, René (2) 17:50

*1: Fraunhofer ITWM, Germany*
*2: RPTU Kaiserslautern-Landau*

Robust PDE-constrained optimizationn requires accounting for uncertainties in model parameters or data. We explore how Polynomial Chaos Expansion enables to perform uncertainty quantification for such problems. This reduces to optimizing with respect to a system of coupled PDEs which admits for the usage of pre-existing solvers. The natural model hierachy induced by the PCE-degree motivates space-mapping strategies for faster optimization. We discuss computational challenges toward high-dimensional uncertain parameters with the goal of analysing robustness for fiber-spinning problems.

**An alternating optimization approach for robust optimal control in chromatography**

Quehl-Cebulla, Dominik H. (1); Gilch, Andrea (2); Rolfes, Jan (3); Kirches, Christian (1); Liers, Frauke (2)

*1: Technische Universität Braunschweig, Germany*
*2: FAU Erlangen-Nürnberg, Germany*
*3: Linköping University, Sweden*

18:10

Chromatographic separation plays a vital role in various areas, as this technique can deliver high-quality products both in lab- and industrial-scale processes. Care must be taken when optimizing such processes, as even small perturbations in the operating conditions can result in significantly altered results, eventually leading to the disposal of the whole product.

In this talk, we propose an algorithmic approach for the robust optimization of chromatographic processes, where we circumvent solving computationally intractable robust mixed-integer optimal control problems constrained by partial differential equations (PDEs) by alternately solving PDE-constrained optimal control problems and distributionally robust optimization problems. Specifically, we split the nominal optimization of the separation process from the robustification of the fractionation times, i.e., the time window where the eluting mass is collected.

We apply our proposed methodology to a realistic case study where a single component is to be separated from two enclosing impurities. We show that our approach indeed generates optimized controls and fractionation times that lead to a robust separation, while requiring only a small number of iterations.

## S19.03: Data-driven methods

Date: March 18, 2026 08:30–09:30
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Recovery of the optimal control value function in reproducing kernel Hilbert spaces from verification conditions**

Ehring, Tobias (1); Azmi, Behzad (2); Haasdonk, Bernard (1)

*1: University of Stuttgart, Germany*
*2: University of Konstanz, Germany*

08:30

Generating accurate approximations of the optimal value function $v^*$ for infinite-horizon, nonlinear, autonomous optimal control problems remains challenging: in general, few algorithms are available that come with rigorous convergence guarantees. Yet obtaining such an approximation is central to real-time synthesis of optimal feedback laws.
We develop an abstract optimal-recovery framework in reproducing kernel Hilbert spaces (RKHS) for reconstructing an unknown target function from mixed equality and inequality functional constraints. Within this framework, approximating $v^*$ is formulated as a collocation-type problem derived from standard verification conditions for optimality—most notably the Hamilton–Jacobi–Bellman (HJB) equation, together with positivity/positive-definiteness requirements—which uniquely characterize $v^*$. As the set of collocation points becomes dense in the domain $\Omega$, we can prove convergence of the resulting RKHS approximants to $v^*$ in two regimes, depending on the assumptions on $v^*$: (i) global convergence on $\Omega$ in the RKHS norm when $v^*$ is analytic, and (ii) local convergence (in a neighborhood of the origin) in the RKHS norm when $v^*$ admits quadratic upper and lower bounds.
We further show that a practical numerical instantiation of the abstract scheme, based on Gauss–Newton linearization, yields an algorithm that reduces to a classical policy-iteration–type method.

Finally, we present four numerical experiments – including a 50-dimensional nonlinear benchmark – that support the effectiveness and scalability of the proposed approach.

**On Koopman operators for time dependent systems**

Winterhager, Tobias; Breiten, Tobias; Hosfeld, René 08:50
*TU Berlin, Germany*

The Koopman operator framework has emerged as a powerful tool for analyzing nonlinear dynamical systems. Its ability to transform complex, nonlinear behaviors into linear evolution has made it increasingly popular across engineering, physics, and data science. However, a significant limitation of the classical Koopman framework is that it relies on time-invariance of the underlying system to obtain semigroup properties, thereby preventing a direct application to (open-loop) controlled systems. One remedy is to resort to an abstract bilinear infinite-dimensional system formulation but this prevents from exploiting linear control concepts.
In this talk, we therefore extend the classical Koopman framework to time-dependent dynamical systems. We analyze the flow induced by such systems and introduce two evolution families acting on observables and densities defined over a bounded domain $\Omega$. For both families, we establish the existence of time-dependent generators, derive explicit representations, and show that the evolution families solve the associated infinite-dimensional linear systems.
As an application, we consider finite-horizon optimal control problems and derive an operator Lyapunov equation characterizing the optimal cost.

**Machine learning methods with a posteriori error analysis for an optimal control problem**

Vossen, Georg; Friedlich, Nicolai; Sirin, Semih 09:10
*Niederrhein University of Applied Sciences, Germany*

We consider an optimal control problem subject to a partial differential equation and present two numerical solution methods based on machine learning which provide surrogate models. Both methods are utilized with a posteriori error analysis for the optimal control where the error can be estimated after the computation of the solution with knowledge of the adjoint state variable. By iteratively increasing the size of the surrogate models, the solution can be obtained with ensured error in the control.

The first method is a Physics-Informed Neural Network (PINN) approach. PINN is a framework used for solving partial differential equations and has also been adopted for optimal control problems by some authors. Here, we use the idea of including penalty terms for the differential equation with boundary and initial conditions, the constraints, as well as the optimization cost functional into the loss function simultaneously. The error estimator is used to determine the transition from a stochastic to a deterministic optimization strategy.

The second approach applies Model-Based Reinforcement Learning (MBRL) to solve the optimal control problem. MBRL is a data efficient method for finding optimal controls often used in, e.g., robotics or game strategies. We use a variant with a probabilistic neural network, radial basis function controller and trajectory sampling. The error estimator is applied in an outer loop of increasing the surrogate model size.

The methods are compared with each other as well as with classical model reduction techniques. The effectiveness of the two approaches will be illustrated with numerical tests.

## S19.04: Shape and topology optimization

Date: March 18, 2026 14:00–16:00
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Shape optimization problems with non-smooth PDE constraints: Sensitivity analysis and optimality conditions**

Betz, Livia 14:00
*Wuerzburg University, Germany*

This talk is concerned with the optimal shape design of non-smooth PDEs. The main particularity of the state system is the lack of differentiability of the underlying nonlinearity. We work within a functional variational approach that has the capacity to transfer geometric optimization problems into optimal control problems, the set of admissible shapes being parametrized by a large class of continuous mappings.

In the first part, we are mainly concerned with the sensitivity analysis of the state equation. We emphasize that we do not resort to extensions on the hold-all domain or any kind of approximation of the original PDE. The computation of the directional derivative of the state w.r.t. functional variations results in a new way of computing the shape derivative. We also introduce the concept of locally optimal shapes and we put into evidence its connection to locally minimizers of the corresponding control problem. With directional differentiability results for the control-to-state map at our disposal, we can then state first-order necessary conditions for locally optimal shapes in general non-smooth settings.

The focus of the second part of the talk is to derive optimality systems that feature an adjoint state. In this context, we present an alternative approach, based on a convex approximation scheme for our original non-smooth shape optimization problem. This permits us to show that each parametrization associated to the optimal shape is the limit of global optima of non-smooth distributed optimal control problems. The admissible set of the approximating minimization problems is a convex subset of a Hilbert space of functions. Its structure is such that one can derive optimality systems by resorting to optimal control theory techniques. This allows us to obtain, via a limiting procedure, sharp first-order necessary optimality conditions for the original non-smooth design problem in the form of a qualified optimality system.

**Long-time behavior of solutions to shape optimization problems via phase-field methods**

Hinze, Michael; Kahle, Christian; Simon, John 14:40
*University of Koblenz, Germany*

We investigate the long time behavior of solutions to a shape and topology optimization problem with respect to the time dependent Navier–Stokes equations. The sought topology is represented by a stationary phase field, that represents a smooth indicator function. The fluid equations are approximated by a porous media approach and are time dependent.
We prove, that if the time horizon tends to infinity, minima of the time dependent problem convergence towards minima of the corresponding stationary problem in the sense that the objective values converges. Also a convergence rate with respect to the time horizon is analytically derived. We validate our results by numerical investigation.

**The impact of the discretization on shape and topological sensitivities**

Gfrerer, Michael (1); Gangl, Peter (2) 15:00
*1: TU Graz, Austria*
*2: RICAM, Austria*

We investigate how the discretization of PDE constraints influences shape and topological derivatives. As a model problem, we study a tracking-type functional together with a two-material Poisson equation in one spatial dimension. In this setting, we analyze the effect of basis function smoothness, and the role of interface resolution. Furthermore, we compare the optimize-then-discretize and discretize-then-optimize approaches.
For the discretization, we use splines of degree p, which provide direct control over basis function smoothness; for example, p=1 yields the usual $C^0$ hat functions. We distinguish between a *standard*

*method* and an enriched method. The standard method does not incorporate interface locations, whereas the enriched method extends the approximation space with enrichment functions that explicitly capture the interface.
For both discretization strategies, we perform shape and topological sensitivity analyses. Our results demonstrate that the regularity of the shape derivative depends on the smoothness of the basis functions, and that pointwise convergence of the shape derivative requires representing the interface in the ansatz space. In contrast, for the topological derivative, convergence is obtained only with the enriched method.

**Optimal Design of Kirchhoff–Love Plates Using Shape Derivatives and Homogenization**
Crnjac, Ivana (1); Jankov Pavlović, Jelena (1); Kunštek, Petar (2)
*1: School of Applied Mathematics and Informatics, University of Osijek, Croatia*
*2: Faculty of Science, University of Zagreb, Croatia*
15:20

We study an optimal design problem for thin elastic plates described by the Kirchhoff–Love model under transverse loading. The objective is to minimize compliance by optimizing both the outer boundary of the plate and the distribution of two isotropic materials within the domain.
Our approach combines shape calculus and homogenization theory within a unified numerical framework. Shape derivatives are employed to guide the evolution of the plate boundary through a level set method, while material optimization in the interior relies on optimality conditions derived from homogenized compliance minimization.
The resulting hybrid algorithm is validated through numerical simulations that demonstrate its accuracy and effectiveness in capturing optimal configurations.

**Classical Optimal Designs for Stationary Diffusion with Multiple Phases**
Vrdoljak, Marko (1); Grbac, Matko (1); Ivec, Ivan (2)
*1: University of Zagreb, Faculty of Science, Croatia*
*2: University of Zagreb, Faculty of Metallurgy, Croatia*
15:40

We study optimal design problems for stationary diffusion involving one or more state equations and mixtures of an arbitrary number of anisotropic materials. Since such problems typically do not admit classical solutions, we adopt a homogenization-based relaxation framework.
The objective considered is the maximization of a weighted sum of the energies associated with each state equation, with particular emphasis on identifying cases in which the optimal design is classical, that is, of bang-bang type, composed solely of the original pure materials. Such cases provide valuable benchmarks for numerical methods in optimal design.
A simplified optimization problem expressed in terms of local material proportions is analyzed through a dual formulation in terms of fluxes. Using a saddle-point characterization, we establish a complete description of its optimal solutions. The proposed approach is applied in detail to spherically symmetric problems. In the case of a ball, the method yields explicit classical solutions of the homogenization-based relaxation problem.

## S19.05: Non-smooth problems
Date: March 18, 2026 16:30–18:30
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Control in the coefficients of the obstacle problem**
Simon, Nicolai; Wollner, Winnifried
*Universität Hamburg, Germany*
16:30

Within this talk, we will discuss the optimal control of an obstacle problem by the choice of the coefficients. To cope with the product in the main part of the operator, tools from H-convergence will be used; see, e.g., [1]. Furthermore, we discuss first-order optimality conditions obtained by extending

a limiting approach for the control of the obstacle problem to the right-hand side, see, e.g., [2,3]. The results are published in [4].


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**A numerical solution approach for non-smooth optimal control problems based on the Pontryagin maximum principle**


Wachsmuth, Daniel 16:50
*University of Wuerzburg, Germany*


We consider nonsmooth optimal control problems subject to a semilinear elliptic partial differential equation
with homogeneous Dirichlet boundary conditions. It is well-known that local solutions satisfy the Pontryagin maximum principle. In this note, we will investigate an optimization method that is based on the
maximum principle. We prove that the discrepancy in the maximum principle vanishes along the resulting
sequence of iterates. Numerical experiments confirm the theoretical findings.

**Chattering solutions for parabolic boundary control problems with terminal observation**


Christof, Constantin 17:10
*Technische Universität Darmstadt, Germany*


We study a parabolic boundary control problem with one spatial dimension, control constraints of box type, and an objective function that measures the $L^2$-distance to a desired terminal state. It is shown that, for a certain choice of the desired state, the considered problem possesses an optimal control that is *chattering*, i.e., of bang-bang type with infinitely many switching points and a positive objective function value. Whether such a solution is possible has been an open question in the literature. We are able to answer this question in the affirmative by means of Fourier analysis and an auxiliary result on the existence of power series with a certain structure and sign-changing behavior. The latter is also of independent interest.

**Derivatives of solution operators of sweeping processes**


Brokate, Martin 17:30
*TU München, WIAS Berlin, Germany*


Solution operators of rate-independent evolutions (in particular, sweeping processes) are typically nonsmooth. We present several results concerning their weak differentiability, including variational characterizations of their directional derivatives. We also discuss applications to optimal control.

**The Latent Variable Proximal Point Algorithm for Optimal Control Problems**
Haaf, Nico 17:50
*IWR Heidelberg, Germany*

We consider several classes of optimal control problems and present a numerical algorithm for their solution, based on the latent variable proximal point algorithm (LVPP). We discuss preconditioning and present numerical results.

**On the Acceleration of Polyak's Heavy-Ball Method**
Kassing, Sebastian (1); Weissmann, Simon (2) 18:10
*1: Universität Wuppertal*
*2: Universität Mannheim*

In this talk, we study the convergence of Polyak's heavy-ball method, in both continuous and discrete time, for general non-convex objective functions. Under the sole assumption that the objective satisfies the Polyak–Łojasiewicz (PL) inequality, we recover the classical convergence rates known for strongly convex functions. In the continuous-time setting, our guarantees hold globally for all initializations. In contrast, in discrete time we perform a local analysis in a neighborhood of the global minimizers. Our results show that the heavy-ball method indeed achieves local acceleration on the class of PL functions. This acceleration also appears in the discrete-time algorithm, provided the iterates enter a sufficiently small neighborhood of the global minima.

## S19.06: Applications
Date: March 19, 2026 08:30–10:30
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Consensus-based Optimization for Boundary Value Problems**
Khatab, Mahmoud; Totzeck, Claudia 08:30
*Wuppertal University, Germany*

Reaching the global minimum cost value without getting stuck in local minima is a challenging task. The contribution of metaheuristic techniques in the last few decades has been significant, providing algorithms capable of finding good approximations of unknown solutions. These approximations are sufficiently accurate and acceptable in engineering applications.
In these algorithms, we seek the solution intelligently by considering a specific indicator, namely the cost function value of agents at their positions. Swarm intelligence (SI) algorithms, such as particle swarm optimization (PSO), ant colony optimization (ACO), and other algorithms [1], are bio-inspired metaheuristic methods. Although such algorithms are powerful tools in optimization, they have not been deeply studied from a mean-field perspective, as most studies focus on numerical results and cost reduction. The Consensus-Based Optimization (CBO) method [2,3] was introduced as a novel approach to trace convergence behavior. In our new approach we are extending the CBO to optimization in infinite dimensional spaces. The power of our new technique is that, with this technique we can approach the very difficult class of boundary problems with state constraints.

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[1] Gendreau, M., & Potvin, J.-Y. Handbook of Metaheuristics, 3rd edition. International Series in Operations Research & Management Science, vol. 272. Springer, 2019.

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[3] Carrillo, J. A., Choi, Y.-P., Totzeck, C., & Tse, O. "An analytical framework for consensus-based global optimization method." Mathematical Models and Methods in Applied Sciences, 28 (2018), 1037–1066.

**Optimal Control of Vlasov-Poisson Models Using the Jensen-Shannon Distance**

Bartsch, Jan (1); Borzi, Alfio (1); Hervieux, Paul-Antoine (2); Manfredi, Giovanni (2)

*1: Universität Würzburg, Departement of Mathematics, Germany*
*2: Institut de Physique et Chimie des Matériaux de Strasbourg, France*

08:50

The Vlasov-Poisson equation describes the evolution of plasmas in the so-called collisionless regime while taking the self-consistent fields into account. The investigation of plasma that is influenced by an exterior magnetic field is a significant aspect in various research fields, ranging from hot to cold plasmas.
One of them is the cooling of plasmas. The adiabatic cooling of non-neutral plasma can be achieved by slowly decreasing the trapping frequency and letting the plasma occupy a larger volume.
In this talk, we propose an optimal control approach within the Lagrange framework for non-adiabatic cooling for plasma trapped in a one-dimensional well. In this approach, the governing model is the Vlasov-Poisson equation and a functional containing the Jensen-Shannon divergence has to be minimized subject to this model constraint and the action of a varying trapping frequency.
A particle method and a gradient-based technique are developed to solve the resulting kinetic optimal control problem.
We present results of numerical experiments that successfully validate the proposed optimal cooling framework with comparing it to the adiabatic cooling.

**Flow of Gas Mixtures in Networks: Modeling and Multi-Objective Optimization**

Ulke, Alena (1); Schuster, Michael (2); Göttlich, Simone (1)

*1: University of Mannheim, Germany*
*2: Friedrich-Alexander University Erlangen-Nürnberg, Germany*

09:10

As climate change necessitates a transition away from fossil fuels, hydrogen emerges as a promising alternative. Additionally, hydrogen-natural gas mixtures provide a viable interim strategy for reducing greenhouse gas emissions. As a result, there is a growing interest in modeling and optimizing the flow of these mixtures in networks. Operating these networks requires satisfying physical and safety constraints while balancing multiple objectives, such as maximizing profit, minimizing costs, increasing the hydrogen share, or reducing emissions, which often conflict with each other.
To address these challenges, we present a mathematical model, the so-called mixture model, that describes the flow of gas mixtures in networks. The model is based on the physical principles of the isothermal Euler equations and the mixing of incoming flow at nodes. Building on this model, we formulate a framework for multi-objective optimization problems that reflect the competing objectives occurring in gas network operation. This framework allows us to compute optimal compromises between the objectives and we show that for a certain class of objectives such optimal compromises exist. We also provide a numerical example to showcase the effectiveness of the proposed idea

**Analysis and Optimal Control of Nonlocal Age- and Space-Structured SVIR Models**

Azmi, Behzad (1); Schlosser, Nicolas (2)

*1: Universität Konstanz*
*2: FAU Erlangen-Nürnberg, Germany*

09:30

Epidemic modeling has long been an important field of research, and the recent Covid-19 pandemic has shown its importance to everyday life. Often, in order to increase accuracy and applicability of the models, a PDE approach is used, thus allowing for modeling spread of infections over countries or accounting for age-depend model parameters such as mortality, infectivity, etc. In this talk, we study a class of nonlinear epidemic models with age and space structure and nonlocal infection terms and introduce an additional control parameter interpreted as a vaccination rate. The main obstacle of our model is that due to its structure, it prevents the use of classical compactness theorems. We show under which conditions the existence of an optimal control can be guaranteed nontheless, and derive first-order optimality conditions for the problem. To conclude, we present numerical simulations of the model and discuss their behaviour.

**A Variational View on Constitutive Laws in Parabolic Problems**

Xylander, Espen (1); Schiffer, Stefan (2)
*1: University of Stuttgart, Germany*
*2: left Academia*

09:50

We consider a variational approach to the modelling of viscous fluids. The physical conservation laws of fluid dynamics are posed as side constrains for a functional that measures how much a given flow deviates from the underlying viscous properties of the fluid.

Based on results on anisotropic quasiconvexity, we discuss parameter regimes where we can prove existence of minimisers and where we can recover well-known results through our variational methods.

**Inherent Structure of Data-Driven Elasticity in Hilbert Space**

Gebhardt, Cristian G. (2); Lankeit, Johannes (1); Steinbach, Marc C. (1)
*1: Leibniz Universität Hannover, Germany*
*2: University of Bergen, Norway*

10:10

The data-driven paradigm replaces classical material laws by a proximity requirement with respect to a set of raw measured strain-stress pairs, thus replacing the standard PDE boundary value problem by a discrete-continuous PDE optimization problem. We treat Dirichlet, Neumann and mixed boundary data in arbitrary spatial dimension and develop a rigorous common framework for classical and data-driven problem formulations. Our Hilbert space setting highlights the inherent problem structure, which is characterized by orthogonal decompositions of several spaces to construct a certain duality of the gradient and divergence operators. The duality arises when regarding grad and div as bounded *and* unbounded operators with respect to suitable norms. Considering linear kinematics, hence linear PDEs, we arrive at a universal unconstrained optimization problem for auxiliary strains and stresses whose solution determines unique physical strains, stresses and deformations and unique dual fields (Lagrange multipliers) associated to the PDE constraints.

## S19.07: Problems on manifolds

Date: March 19, 2026 14:00–16:00
Room: KII, M17.92
Chair(s): Azmi, Behzad
Schaller, Manuel

**Newton methods for variational problems on nonlinear spaces**

Schiela, Anton (1); Weigl, Laura (1); Bergmann, Ronny (2)
*1: Universität Bayreuth, Germany*
*2: Norwegian University of Science and Technology, Norway*

14:00

An important class of nonlinear PDEs can be formulated as variational problems on nonlinear spaces, such as Hilbert manifolds. To solve these problems efficiently Newton's method can be applied.
In this talk we will discuss Newton methods for mappings between nonlinear manifolds. Of particular interest are variational problems, which can be formulated via mappings from a manifold into a dual vector bundle. To render Newton steps well defined in this setting, we have to equip the vector bundle with a connection.
We will discuss local convergence and provide some numerical examples.

**Optimal control of PDEs for mappings into manifolds**

Weigl, Laura; Schiela, Anton
*University of Bayreuth, Germany*

14:20

In this talk, we consider optimal control problems with partial differential equation (PDE) constraints involving mappings into manifolds. This class of problems differs from the classical setting of linear spaces in various ways.

Specifically, the treatment of variational problems on manifolds requires the use of special techniques. We derive optimality conditions and discuss the application of Newton's method for their numerical solution. As application, we present the optimal control of an elastic geodesic by a force field.

**Optimal design with inverse deformation analysis and stress constraints**

Gartner, Dominik; Gfrerer, Michael H. 14:40
*Technische Universität Graz, Austria*

In many engineering applications, achieving a prescribed deformed configuration is a central design objective. We consider inverse deformation analysis, aiming to recover the undeformed shape corresponding to a given deformed configuration under known loads such as body forces or shrinkage. A key contribution is the rigorous derivation of the deformation gradient for the inverse Eulerian problem. This formulation enables an efficient finite element implementation while maintaining numerical stability at finite strains. Numerical examples demonstrate that the undeformed configuration can be recovered from the deformed state in a single iteration. The result is validated by a corresponding direct control simulation.

Building on this framework, we address shape optimization problems with partially prescribed deformed boundaries. The inverse deformation problem serves as the state equation, while free boundaries are optimized to minimize material usage subject to stress constraints. This results in a robust approach for the design and optimization of structures directly in their deformed configuration.

The complete workflow is implemented in AutoFreeFEM, enabling concise problem specification and reproducible results within the FreeFEM environment.

**Riemannian gradient descent along geodesic paths for shape optimization using isogeometric analysis**

Rosandi, Rozan; Simeon, Bernd 15:00
*RPTU Kaiserslautern-Landau, Germany*

A common procedure in isogeometric shape optimization is to use a NURBS description of the geometry and consider a subset of control point coordinates as design variables [1, 2, 3], which corresponds to the first discretize–then optimize approach. While this is a fairly straightforward way to perform shape optimization in the context of isogeometric analysis, the results will usually depend on the particular representation of the geometry, since the problem is reduced to a finite-dimensional one that often disregards the inherent geometric structure of shapes. We present the Riemannian framework for PDE constrained shape optimization [4] in an attempt to provide suitable descent paths for control points that evolve the shape in a consistent manner independent of the chosen representation. The idea is to endow the shape space with a reparametrization-invariant Riemannian metric [5] and move the shapes along geodesic paths corresponding to the metric, which allows for mesh-independent shape optimization. This first optimize–then discretize approach has been applied to the compliance minimization of thin elastic shells using a first-order Sobolev-type metric in [6]. We now investigate the effects of using geodesic retractions for optimization on Riemannian shape spaces of planar curves and surfaces, where isogeometric finite element methods are used for the discretization of the equations to efficiently obtain accurate numerical approximations of the Riemannian shape gradient.

References:

[1] W. Wall, M. Frenzel, and C. Cyron. Isogeometric structural shape optimization. Computer Methods in Applied Mechanics and Engineering, 197:2976–2988, 2008.
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[3] J. Lopez, C. Anitescu, and T. Rabczuk. Isogeometric structural shape optimization using automatic sensitivity analysis. Applied Mathematical Modelling, 89:1004–1024, 2021.
[4] V. H. Schulz, M. Siebenborn, and K. Welker. PDE constrained shape optimization as optimization

on shape manifolds. In F. Nielsen and F. Barbaresco, editors, Geometric Science of Information, volume 9389 of Lecture Notes in Computer Science, pages 499–508. Springer, 2015.
[5] M. Bauer, P. Harms, and P. W. Michor. Sobolev metrics on shape space of surfaces. Journal of Geometric Mechanics, 3(4):389–438, 2011.
[6] R. Rosandi and B. Simeon. Riemannian shape optimization of thin shells using isogeometric analysis. Proceedings in Applied Mathematics and Mechanics, 25(1):e202400204, 2025.

## S20: Dynamics and control

Organizer(s): Köhler, Johannes *(ETH Zurich)*
Iannelli, Andrea *(University of Stuttgart)*

## S20.01: Applications I

Date: March 17, 2026 08:30–10:30
Room: KII, M17.17
Chair(s): Ströhle, Timo
Wembe, Boris

### Cayley Based-Methods for Quantum Optimal Control Systems

Wembe, Boris (1); Ali, Usman (2); Meier, Torsten (1); Ober-Blöbaum, Sina (1) 08:30
*1: Paderborn University, Germany*
*2: Carl von Ossietzky Universität, Germany*

Accurate simulation and control of quantum systems require numerical schemes that respect the physical structure of the underlying equations. When quantum dynamics are simulated with standard numerical integrators, such as Runge–Kutta or splitting methods, they may accumulate small errors that eventually destroy key invariants, in particular unitarity, the mathematical expression of probability conservation. In large-scale quantum control problems, where thousands of propagations are needed to optimize laser pulses or field parameters, these numerical errors can become a serious limitation.
In this talk, I will present a new family of structure-preserving integrators based on the Cayley commutator-free (CF–Cayley) formulation. The central idea is to replace expensive matrix exponentials by Cayley transforms, simple linear solves that automatically evolve on the unitary manifold, while avoiding nested commutators. This yields algorithms that are fast, symmetric, and exactly norm-preserving, making them ideally suited for repeated forward and backward propagations in optimal control algorithms such as Krotov's method.
Beyond quantum control, this approach provides a general framework for the geometric integration of differential equations on Lie groups, bridging ideas from applied mathematics, physics, and numerical analysis. It demonstrates how respecting the underlying geometry of a system, rather than merely discretizing its equations, can lead to both deeper insight and practical computational gains.

### Modelling and Implementation of Continuous Optimal Power Flow for Optimality-Tracking

Chen, Shuo (1,2); Heilscher, Gerd (1); Urban, Karsten (2) 08:50
*1: Ulm University, Germany*
*2: Ulm University of Applied Sciences, Germany*

In the era of energy transition and digitalisation, the application of numerical methods for solving Optimal Power Flow (OPF) problems is an essence. In practice, OPF models are formulated as discrete, static optimisation problems in a "first discretise, then optimise" sense. This approach has severe limitations, e.g. concerning time steps, data assimilation and stability.

In that regard, this talk focuses on modelling and implementation of a continuous OPF (COPF) approach that is designed to track the known optimality condition. Following the concept of "Prediction-Correction Interior Point Method" (PC-IPM) introduced in [1], the necessary first-order condition is shown to be an ODE system. The COPF model is based upon two assumptions: 1) at discrete time points, optimal power setpoints of controllable generators can be determined by a static OPF; 2) data are available at each discrete time point, and the intermediate data can be smoothly approximated by polynomial interpolation. The main challenge is that the right-hand side of the ODE is not a simple, explicitly prescribed symbolic function, but rather a complex expression involving three derivative terms of a time-dependent function. We suggest to use Algorithmic Differentiation for an efficient solution of this ODE.

Using the known optimality at a fixed timestep as initial condition, different methods of numerical integration were applied to the Initial Value Problem (IVP) to obtain solution trajectories, which turned

out to be extremely sensitive to the parameters appearing in the ODE. Moreover, by introducing a small second-order derivative term multiplying a perturbation parameter, one can incorporate another known optimality condition at the terminal time point. Consequently, the IVP is transformed into a perturbed Boundary Value Problem (BVP), [2]. This allows us to determine a solution trajectory that satisfies the two boundary conditions while preserving sub-optimality over the entire interval.

Using static OPF solutions computed by MATPOWER on a finely discretised time mesh as reference, we present numerical results for solving the COPF in the IVP and BVP setups.

[1] Mahyar Fazlyab et al. “Interior point method for dynamic constrained optimization in continuous time”. In: 2016 American Control Conference (ACC). ISSN: 2378-5861. July 2016, pp. 5612–5618

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**Model Predictive Control for ergodic information acquisition in marine environment**

Pisciolini, Caterina (1,2); Bucci, Alessandro (2); Ridolfi, Alessandro (2); Flaßkamp, Kathrin (1) 09:10
*1: Saarland University, Germany*
*2: University of Florence, Italy*

This presentation addresses active information acquisition in fluvial and marine environments. Classical strategies from literature tend to separate the problems of coverage and target localization. Lawnmower paths are simple and easy to implement for underwater monitoring missions, but they have notable limitations. It is necessary to assume uniform coverage requirements and a largely static environment, which makes it inefficient in dynamic or heterogeneous areas. Moreover, it is not possible to handle accurate or focused inspection of specific areas of interest, as it lacks adaptability in path resolution. Contrarily, we propose a Model Predictive Control (MPC) approach using ergodicity metrics as cost functions. The optimization-based problem setting of finite-horizon MPC allows to determine suitable trajectories for nautical
vehicles. This is ensured by the integration of the dynamic model of a vessel or underwater vehicle including kinematics constraints within the control algorithm. Due to the limited agility of nautical vehicles, a suitable choice of the MPC prediction horizon is of importance. Moreover, ergodicity costs have to be balanced with the control effort. Thus we include a second control cost and analyze the multiobjective optimization problem. The exploration of ergodicity for efficient search has already been explored for Unmanned Aerial Vehicles (UAVs) and for bio-inspired robots in marine environment within literature. Our simulative results are based on a direct method for solving the optimal control problems within MPC, together with a Fourier series approximation of the probability density functions modeling the information.

**Dynamic Feed-Forward Model-Based Control of a Soft Robot Using Servo Constraints**

Dielhenn, Jana; Grube, Malte; Seifried, Robert 09:30
*Technische Universität Hamburg, Germany*

The relatively young field of soft robotics comprises a wide spectrum of disciplines ranging from material science to modeling and actuation of highly dynamical systems. In distinction to conventional robots manufactured from stiff and rigid components, soft robots are made from flexible and soft materials like silicone enabling large deformations. Their high flexibility and adaptability make soft robots destined for delicate tasks found e.g. during human-machine interaction or the handling of sensitive objects. Due to these properties, soft robots find application in various fields, such as the medical sector or fruit harvesting. As most soft robots deform continuously, a large number of degrees of freedom arises making soft robots predominantly underactuated and oftentimes redundantly actuated. These unique properties pose new challenges especially in modelling and control. As a result, most soft robotic applications are currently limited to slow motions or fields with low accuracy requirements. Common opposed control approaches currently found in the field of soft robotics include so-called kinematic vs. dynamic, model-based vs. model-free or open- vs. closed-loop controllers. Kinematic controllers neglecting inertia and damping effects are used for slower motions, hence also rereferred to as quasi-static controllers. In contrast to that, dynamic controllers do account for these

effects. In soft robotics, data-based models are categized as model-free as opposed to model-based. Closed-loop control concepts in soft robotics are mostly limited by the required sensor feedback. While external camera tracking systems can be utilized in an academic setting, this is often not practical for real-world application. Soft sensors that can directly be integrated into soft robots have thus to be developed. Alternatively, open-loop control solely relying on an accurate model of the soft robot rather than sensor feedback can be added to a closed-loop controller or even exclusively employed in order to decrease sensor demands. Prevailing control concepts for soft robots are predominantly quasi-static and therefore omit relevant dynamic phenomena. Dynamic concepts do exist but are primarily data-driven and rely on prior training to execute predefined tasks.

In order to allow for accurate dynamic trajectory tracking of fast motions, this contribution presents an open-loop model-based dynamic trajectory tracking control strategy for a tendon-actuated beam-shaped soft robot using servo-constraints. The soft robot is modeled using piecewise constant curvature (PCC) enabling the inclusion of dynamic effects. Because of the open-loop control concept, no internal or external sensors or tracking systems are required. First experimental results show the strength of this approach.

**Learning preferenced paths in street graphs via weight identification**

Paulus, Matthias Jochen; Flaßkamp, Kathrin
*Universität des Saarlandes, Germany*

09:50

Conventional mobility analysis strategies for street networks rely on a mix of local measurements and statistical surveys to estimate traffic flows and travel patterns.
However, modern data sources, such as traffic participants' trajectories, provide new opportunities to analyze mobility patterns at a large scale.
In this talk, we model traffic participants' trajectories in a street network, i.e., a graph.
Optimal paths in a graph can be obtained via combinatorial solvers, since this task belongs to the class of discrete optimization problems.
Combinatorial solvers find optimal solutions by minimizing a cost function that is defined as the sum of the weights of the utilized edges
However, in many real-world applications, modelling the weights is a difficult choice, though.
This is because weights are generally not directly observable, even under the assumption that a large quantity of participant trajectories as percepted-to-be optimal solutions are available.
In this talk, we propose a framework to identify weights in a graph from a set of optimal solutions, using the example of a street network and the corresponding paths taken by traffic participants. The framework relies on a method of gradient estimation for combinatorial solvers in order to apply methods from unconstrained optimization.

**Modelling and control of pressure-driven flow within compliant microfluidic capillaries**

Ströhle, Timo (1); Petit, Nicolas (2)
*1: Karsruher Institut für Technologie, Germany*
*2: Mines Paris, Université PSL, France*

10:10

In pressure-controlled microfluidics, liquid transport through microchannels is driven by the pressure difference between in- and outlet, and in rigid channels the flow rate is well approximated by a linear pressure–flow relationship set by hydraulic resistance and fluid viscosity. In practice, however, microfluidic systems frequently include compliant elements, most notably elastic channel walls in PDMS devices, but also membranes, valves, tubing, and connectors, that deform under pressure and thereby couple the pressure field to channel geometry. This fluid-structure interaction dynamically alters the cross-sectional area and hydraulic resistance, producing nonlinear and sometimes counter-intuitive transients such as flow-rate overshoot, backflow, and non-monotonic pressure-flow behavior.
Although these effects are primarily transient and the flow typically converges to a predictable steady state once mechanical equilibrium is reached, the associated settling time can disrupt mixing patterns and flow distribution, force repeated flushing, and waste

valuable reagents. This can be particularly costly in biotechnology applications involving scarce or expensive cell types.
Motivated by these challenges, this contribution presents the pressure-controlled dynamics of the outlet flow rate in an elastic microchannel. A linear distributed-parameter model is proposed, from which non-rational transfer functions are derived to characterize the system dynamics. The analysis highlights key features such as high-frequency ringing, echo effects in the step response, and overshoot in the outlet flow rate. Numerical simulations based on the *Method of Characteristics* corroborate the predicted complex transient behavior and are further used to solve the inverse problem of determining the inlet pressure required to achieve a smooth outlet flow rate. Building on this framework, several motion-planning and transient pre-compensation strategies are introduced to suppress ringing and echoes, including optimization-based approaches that explicitly incorporate practical constraints on the magnitude and rate of change of the inlet pressure.

## S20.02: Optimal Control

Date: March 17, 2026 16:30–18:30
Room: KII, M17.17
Chair(s): Köhler, Johannes
Vladimirsky, Alexander

### Towards real-time model predictive control of nonsmooth dynamical systems

Nurkanovic, Armin 16:30
*University of Freiburg, Germany*

Nonsmooth dynamical systems are ubiquitous in many applications, ranging from fast, contact-rich robot dynamics to large-scale processes in engineering that involve phase changes and flow reversals. However, the nonsmooth nature of these dynamics violates the regularity assumptions typically made in the control and optimization of smooth nonlinear dynamic systems.
In this talk, we focus on direct optimal control and real-time model predictive control (MPC) of nonsmooth systems. In a direct approach, we formulate a continuous-time optimal control problem, discretize it in time, and solve the resulting finite-dimensional nonlinear program. In the nonsmooth setting, however, none of the steps in this pipeline can rely on established methods; each requires a fundamentally new approach.
We draw parallels between the well-established algorithmic paradigms that enable real-time MPC for smooth nonlinear systems, and the new ideas required for real-time MPC of nonsmooth systems. The talk covers the full computational pipeline and highlights key innovations from recent years that enable MPC of nonsmooth systems. These developments include novel reformulations, particularly the transformation into computationally favorable dynamic complementarity systems, new time-discretization methods that allow exact derivative computation, switching detection, and high accuracy, as well as new optimization algorithms and their efficient implementations for real-time nonsmooth optimization problems.
The concepts are illustrated through both tutorial examples and challenging benchmark problems.

### Optimality and Robustness in Path-Planning Under Initial Uncertainty

Qi, Dongping (1); Dhillon, Adam (2); Vladimirsky, Alexander (1) 17:10
*1: Cornell University, United States of America*
*2: University of California, Berkeley, United States of America*

Classical deterministic optimal control problems assume full information about the controlled process. The theory of control for general partially-observable processes is powerful, but the methods are computationally expensive and typically address the problems with stochastic dynamics and continuous (directly unobserved) stochastic perturbations. In this presentation we focus on path planning problems which are in between – deterministic, but with an initial uncertainty on either the target or the running cost on parts of the domain. That uncertainty is later removed at some time $T$, and the goal is to choose the optimal trajectory until then. We address this challenge for three different models

of information acquisition: with fixed *T*, discretely distributed and exponentially distributed random *T*. We develop models and numerical methods suitable for multiple notions of optimality: based on the average-case performance, the worst-case performance, the average constrained by the worst, the average performance with probabilistic constraints on the bad outcomes, risk-sensitivity, and distributional-robustness. We illustrate our approach using examples of pursuing random targets identified at a (possibly random) later time *T*.

**LPV Updates for Sequentially Linearized Moving Horizon Estimation of Nonlinear Systems**

Ji, Jiaxin (1); Heiland, Jan (1); Karachalios, Dimitrios (2); Abbas, Hossam (2)

*1: TU Ilmenau, Germany*
*2: University of Lübeck, Germany*

17:30

Moving Horizon Estimation (MHE) provides high precision state estimation for nonlinear systems, but it is often limited by the substantial computational demands of solving a nonlinear optimization problem at every sampling step.

To address this issue, and considering the recently developed approach in [1], we develop an efficient MHE scheme based on a Linear Parameter-Varying (LPV) formulation, where the scheduling parameter is given by the estimated states of the system and used to update inexact Hessians and gradients/ Jacobians used in the Quadratic Programming(QP) subproblem.

Nonlinear MHE problem is first expressed in a LPV form, in which the nonlinear dynamics are expressed as a parameter-dependent linear structure. Based on this LPV representation, Karush–Kuhn–Tucker (KKT) conditions associated with the Nonlinear Programming (NLP) of the MHE optimization problem are approximated and formulated in terms of the scheduling parameter and solved using an inexact Newton-type update, leading to a Sequential Quadratic Programming (SQP) framework with a structured QP subproblem at each iteration, which can be systematically updated via the scheduling parameter, eliminating the need to compute gradients or Hessians in each iteration of conventional SQP algorithms for NLP. The resulting SQP-MHE scheme preserves the estimation performance of nonlinear MHE while substantially reducing computation through linear constraints in the LPV model and the quadratic cost formulation.

[1]. Karachalios, Dimitrios S., and Hossam S. Abbas. "Efficient Nonlinear Model Predictive Control by Leveraging Linear Parameter-Varying Embedding and Sequential Quadratic Programming."

**Stability of stochastic economic MPC - Stochastic characterization of the closed-loop asymptotics**

Schießl, Jonas (1); Selder, Hannah (2); Ou, Ruchuan (3); Baumann, Michael Heinrich (1); Faulwasser, Timm (3); Grüne, Lars (1)

*1: University of Bayreuth, Germany*
*2: Leipzig University, Germany*
*3: Hamburg University of Technology, Germany*

17:50

In this talk, we analyze stochastic economic model predictive control (MPC) schemes with an expected cost criterion and establish closed-loop stability guarantees. Building on stochastic turnpike properties and dissipativity concepts, we construct suitable Lyapunov functions that allow us to prove practical asymptotic stability of the MPC closed loop without relying on terminal costs or terminal constraints. In contrast to existing results, we provide an exact characterization of the asymptotic behavior of the MPC closed-loop trajectories in terms of a specific stationary stochastic process. This enables us to provide stability statements on different levels, such as mean square, pathwise in probability, in distribution, or in moments, which are in line with common stochastic convergence concepts.

**On the Design of Terminal Ingredients in Periodic Model Predictive Path-Following**

Abou-Taleb, Mohamed (1,2); Berberich, Julian (1); Zeilinger, Melanie (2); Carron, Andrea (2) 18:10
*1: University of Stuttgart, Germany*
*2: ETH Zürich, Switzerland*

Establishing recursive feasibility and asymptotic stability for nonlinear Model Predictive Path-Following Control (MPPFC) is a non-trivial task, particularly when following periodic reference paths. We propose a procedure for the design of terminal ingredients in MPPFC for constrained nonlinear systems. In MPPFC, the system is augmented by a progress dynamics and a virtual control input, the *progress velocity*, which acts as an additional decision variable in the optimization problem. In contrast to standard time-based tracking MPC, this allows the controller to optimize over the timing associated with the reference. Based on a periodic path in the state space and a nominal timing, we design a periodically time-varying quadratic terminal cost and ellipsoidal terminal region using the linearization along this nominal trajectory. This is achieved by finding a periodic solution to a suitable Riccati differential equation. Crucially, we reparameterize these time-based ingredients in terms of the progress variable, resulting in a progress-varying quadratic terminal cost and ellipsoidal terminal region. Furthermore, we prove that the resulting scheme is recursively feasible, the error dynamics are asymptotically stable, and that the progress velocity converges to the nominal reference.

## S20.03: Applications II

Date: March 18, 2026 08:30–09:30
Room: KII, M17.17
Chair(s): Röbenack, Klaus
Köhler, Johannes

**On the Expectation Values of the Structural Index of Low-Dimensional Random Structure Matrices**

Röbenack, Klaus 08:30
*TUD Dresden University of Technology, Germany*

The qualitative behavior of solutions of differential algebraic equations (DAEs) is primarily characterized by the index. For linear time-invariant DAEs, the index essentially depends on the filling pattern of the matrices involved. To this end, one switches from numerical matrices to structure matrices and computes the structural index for these. The index of a matrix pencil can be reduced to the index of a single matrix.

This contribution addresses the question of how the index typically depends on the filling density of a matrix. For this purpose, it is assumed that the entries of a structural matrix are subject to a Bernoulli distribution. For low-dimensional structural matrices, the expectation value of the structural index can then be calculated as a function of the probability parameter of the Bernoulli distribution.

**Mathematical analysis of Diphtheria epidemic model with vaccination and transport-related infection**

Kanchanarat, Siwaphorn (1); Chinviriyasit, Settapat (2); Chinviriyasit, Wirawan (2) 08:50
*1: Department of Social and Applied Science, College of Industrial Technology, King Mongkut's University of Technology North Bangkok, 1518 Pracharat 1,Wongsawang, Bangsue, Bangkok 10800, Thailand.*
*2: Department of Mathematics, Faculty of Science, King Mongkut's University of Technology of Thonburi, 126 Pracha Uthit Road, Bang Mod, Thung Khru, Bangkok 10140,Thailand*

A diphtheria epidemic model with imperfect vaccination and transport-related infection is formulated. The dynamics of diphtheria transmission are determined by the threshold value of the formulated model, known as the reproductive number, which is defined by $R_m$. It is shown that the disease-free equilibrium is globally asymptotically stable; that is, diphtheria will die out whenever $R_m \leq 1$. When $R_m > 1$, the endemic equilibrium exists and is locally asymptotically stable. Numerical simulations are illustrated with theoretical results and applied to explore the effect of transport-related infection in diphtheria control by vaccination. The results of this study provide useful information to support

decision-making for transport policy during the epidemic period and help address the deficiencies in implementing a vaccination strategy.

**Space-Time Finite Element Method for the Inverse Dynamics of Flexible Structures**
May, Marvin; Ströhle, Timo; Betsch, Peter
*Karlsruhe Institute of Technology, Germany*
09:10

In engineering, the dynamics of flexible structures such as beams or strings are commonly simulated using semidiscretization, a spatial discretization, typically based on the Finite Element Method, combined with a time-stepping scheme. An alternative approach is the simultaneous discretization of the space-time domain. Compared to standard finite-difference schemes, this formulation allows the use of unstructured meshes and enables backward propagation of information in time, which is essential for solving inverse dynamics and optimal control problems.

Inverse dynamics problems can be addressed using servo constraints to obtain feedforward control inputs. However, the resulting differential-algebraic equation (DAE) systems may exhibit rapidly increasing index when solved sequentially. This issue can be avoided through a simultaneous space-time solution strategy. In this contribution, we present a space-time finite element method for solving general initial-boundary value problems as well as inverse dynamics problems. In addition to standard displacement-based finite elements, we employ a mixed Hellinger-Reissner type formulation to mitigate shear locking in the simulation of slender beams.

The planar examples discussed here can be extended straightforwardly to spatial problems. The proposed method is applied to representative flexible structures, and its numerical properties are analyzed in detail.

## S20.04: Optimization for dynamical systems

Date: March 18, 2026 14:00–16:00
Room: KII, M17.17
Chair(s): Iannelli, Andrea
Bongarti, Marcelo

**Structure, Analysis, and Synthesis of First-Order Algorithms**
Miller, Jared; Scherer, Carsten; Fabian, Jakob; Iannelli, Andrea
*University of Stuttgart, Germany*
14:00

Optimization algorithms can be interpreted through the lens of dynamical systems as the interconnection of a stepsize-governing linear system and a set of gradient or subgradient nonlinearities. This dynamical systems formulation allows for the analysis and synthesis of optimization algorithms through the solution of robust control problems. In this work, we use the celebrated internal model principle in control theory to structurally factorize any convergent optimization algorithm into a suitable internal model and a core controller. As the key benefit, we reveal that this permits to synthesize optimization algorithms even if gradient information is transmitted over corrupted networks. Computation of these certified-exponentially-convergent networked algorithms is achieved by solving semidefinite programs under bisection. We demonstrate factorization of existing optimization algorithms and the automated synthesis of new tracking algorithms.

**Asymptotic behaviour of coupled random dynamical systems with multiscale aspects**
Staudigl, Mathias (1); Luke, Russel (2); Peypouquet, Juan (3); Schnebel, Johannes (1); Qu, Siqi (1)
*1: Universität Mannheim, Germany*
*2: Universität Göttingen*
*3: Rijksuniversiteit Groningen*
14:20

We study the asymptotic behaviour of a class of stochastic differential inclusions involving multiscale features. This class of problems allows us to study the long-run properties of set-valued dynamical systems which are confined to remain in the domain of a maximally monotone operator, and asymptotically approach a constrained domain over which an equilibrium is searched for. In particular, our

results contain a class of SDEs with reflection in a convex domain. We establish asymptotic convergence, as well as rates in continuous time, as well as discrete-time using a suitable Euler-Maruyama discretisation. We complement our study with quantifying large-deviations and provide a set of comprehensive numerical examples, illustrating the performance of our method.

**A Stochastic Gradient Descent Approach to Design Policy Gradient Methods for LQR**

Song, Bowen (1); Weissmann, Simon (2); Staudigl, Mathias (2); Iannelli, Andrea (1)
*1: University of Stuttgart, Germany*
*2: University of Mannheim, Germany*

14:40

In this work, we apply a stochastic gradient descent (SGD) framework to design data-driven policy gradient descent algorithms for the linear quadratic regulator (LQR) problem under stochastic dynamics. Stochastic trajectory data are used to estimate the gradient through two schemes: (i) an online identification–based method, in which system matrices are first estimated using recursive least squares (RLS) and subsequently used to construct the gradient, corresponding to indirect data-driven control; and (ii) a zeroth-order method, which directly approximates the gradient via empirical cost evaluations generated from ergodic data, corresponding to direct data-driven control. In both schemes, the estimated gradient naturally acts as a stochastic gradient due to the stochasticity in the data, allowing the application of SGD theory to analyze convergence. We formalize the resulting stochastic gradient estimates from both schemes as gradient oracles. Due to the nonlinear structure of the gradient expression, these oracles are inherently biased.

It is well known that the LQR cost function is nonconvex but satisfies gradient-dominance and quasi-smoothness properties. Leveraging these structural properties, we derive conditions on the step size and bias term under which an SGD-type algorithm equipped with a general biased gradient oracle converges asymptotically to the optimal policy. We then identify the specific conditions under which the indirect and direct gradient estimation schemes satisfy the requirements on the bias term, thereby ensuring that the corresponding data-driven policy gradient descent algorithms converge to the optimal policy, extending existing results in the literature, which typically guarantee convergence only to suboptimal policies. Finally, we use the derived oracle conditions to compare the advantages and limitations of the two data-driven approaches, and numerical experiments illustrate the effectiveness of the proposed methods.

**Stability of Time-Varying Receding Horizon Games**

Erdin, Alexander Casper (1); Hall, Sophie (2)
*1: Hamburg University of Technology, Germany*
*2: ETH Zurich, Switzerland*

15:00

Many real-world systems, such as traffic networks, energy grids, and autonomous vehicles [1, 2, 3], exhibit an inherent game-theoretic structure, as self-interested agents act to optimize their own objectives. These games are often played over very long, sometimes even infinite, horizons, making the computation of their exact solutions impractical. To address this challenge, recent control methodologies approximate the solution in a receding-horizon manner, a framework commonly referred to as game-theoretic model predictive control (MPC) or receding horizon games (RHGs).

In the recent work [4], stability results were established for time-invariant RHGs under a potential-game structure. In this work, we extend these results to the time-varying setting, where the optimal operating behavior is characterized by a time-varying trajectory rather than a steady-state. To accomplish this, we build on the connection between RHGs and economic MPC (EMPC) theory first established in [4], which allows us to derive practical asymptotic stability of the optimal trajectory using recent EMPC results [5]. Consequently, we provide closed-loop stability guarantees for RHGs with time-varying, linear-quadratic objectives, and linear time-varying dynamics.

**References**

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[5] L. Grüne and S. Pirkelmann, “Economic model predictive control for time-varying system: Performance and stability results,” Optimal Control Applications and Methods, vol. 41, no. 1, pp. 42–64, 2020, eprint: https://onlinelibrary.wiley.com/doi/pdf/10.1002/oca.2492. [Online].
Available: https://onlinelibrary.wiley.com/doi/abs/10.1002/oca.2492

**Learning provably bounded polynomial ODEs from data**

Fantuzzi, Giovanni; Alcalde, Albert
*Friedrich-Alexander-Universitaet (FAU) Erlangen-Nuernberg, Germany*

15:20

One of the main challenges in learning dynamic models from data is ensuring their boundedness, meaning that model solutions eventually remain within a bounded "trapping region". The difficulty is that both the model and its corresponding trapping region need to be learned simultaneously, leading to a non-convex optimization problem that is typically difficult to solve. In this talk, I will demonstrate that this challenge can be overcome when learning polynomial ODE models by using a model-free Lyapunov framework to identify trapping regions directly from data. This framework, which integrates *extended dynamic mode decomposition* with polynomial optimization techniques, allows one to separate the "trapping region discovery" step from the "model discovery" step. As a result, each step can be implemented as a tractable semidefinite program, enabling the efficient learning of polynomial ODE models that are not only accurate, but also *provably bounded*. The effectiveness of this method will be illustrated using a variety of examples.

**State constrained convex Nash equilibrium problems coupled with linear hyperbolic PDEs**

Bongarti, Marcelo; Hintermüller, Michael
*Weierstrass Institute for Applied Analysis and Stochastics, Germany*

15:40

Generalized Nash equilibrium problems coupled with PDEs appear in many multi-agent systems with shared dynamics and constraints. While existence results are well established for elliptic and parabolic couplings, the hyperbolic case remains largely open due to the lack of compactness of the strategy-to-state map and the resulting difficulties caused by state constraints. In this talk, we present recent results on convex, state-constrained GNEPs coupled with linear hyperbolic PDEs, explain how equilibrium existence can be proved despite these challenges, and discuss the key structural assumptions behind the analysis. We also outline first-order optimality conditions and show how the framework applies to concrete models such as the wave equation, advertising dynamics, and linearized isothermal Euler systems on networks.

## S20.05: Port-Hamiltonian systems

Date: March 18, 2026 16:30–18:30
Room: KII, M17.17
Chair(s): Iannelli, Andrea
Schaller, Manuel

**Port-Hamiltonian Systems: Opportunities and challenges for analysis, numerics and optimal control**

Schaller, Manuel 16:30
*Faculty of Mathematics, Technische Universität Chemnitz, Germany*

Port-Hamiltonian systems provide a modeling framework for dynamical systems that extends the classical concept of Hamiltonian systems through the introduction of interconnection ports. These ports can be used, for example, to enable control access, to incorporate observations, or to achieve structure-preserving coupling between subsystems. As a result, port-Hamiltonian systems are particularly powerful for the modular modeling of complex dynamical systems. Moreover, a central feature inherited from Hamiltonian systems is that the dynamics are naturally accompanied by a notion of energy, which is dissipated along uncontrolled solutions.

In this talk, we will explore the opportunities arising from these structural properties, including the dissipativity of the underlying operators and how this can be exploited in functional analytic considerations such as well-posedness. We will also discuss numerical aspects for simulation, in particular the efficient solution of the resulting systems by means of tailored preconditioning strategies. However, the preservation and proper treatment of the structure and energetic properties of port-Hamiltonian systems in simulation and optimal control pose significant challenges. These include the need for structure-preserving integration schemes and the occurrence of singular optimal control problems that require approaches beyond standard quadratic control costs.

**Optimization-based control by interconnection of nonlinear port-Hamiltonian systems**

Preuster, Till (1); Schaller, Manuel (1); Gernandt, Hannes (2) 17:10
*1: Chemnitz University of Technology, Germany*
*2: University of Wuppertal, Germany*

Model Predictive Control (MPC) is a well-established optimization-based control strategy, but its real-time implementation often poses significant computational challenges. A way to deal with these challenges are suboptimal MPC approaches, in which the optimal control solver for feedback computation is terminated prematurely.

In this talk, we present a suboptimal MPC scheme for port-Hamiltonian systems. The approach exploits the inherent dissipativity of the optimality system, which arises from its primal–dual structure, together with the dissipativity of the underlying port-Hamiltonian dynamics. This allows us to formulate the MPC scheme as a control-by-interconnection of two port-Hamiltonian systems. Using the dissipativity of the resulting closed-loop system, we establish well-posedness and convergence of the method in function space, thereby showing in particular mesh-independent convergence of the scheme.

**Towards Polynomial Representations of Port-Hamiltonian Systems**

Itani, Mohammad (1); Schaller, Manuel (2); Worthmann, Karl (3); Faulwasser, Timm (1) 17:30
*1: Hamburg University of Technology*
*2: Chemnitz University of Technology*
*3: Technische Universität Ilmenau*

The port-Hamiltonian framework provides a unified modeling approach for many physical systems. Such systems are often nonlinear, which makes the formulation of generic analysis and synthesis approaches very difficult, if not impossible. We propose an alternative polynomial representation for port-Hamiltonian systems that lives in a higher-dimensional space. This representation is obtained via a lifting map, which is also an immersion. We show that the dissipated power in the obtained representation is identical to that of the original system on the range of the lifting map, which in turn defines an invariant manifold. We illustrate our findings with numerical examples. Finally, we demonstrate, through an example, the utility of the polynomial representation in solving control problems for port-Hamiltonian systems via sum-of-squares optimization.

**Dissipativity properties of a class of nonlinear time-delay systems**
Gernandt, Hannes (1); El Haskouki, Ikram (1,2)
*1: University of Wuppertal, Germany*
*2: University of Hassan II Casablanca, Morocco*
17:50

Time delays are inherent in many physical and engineered systems and can significantly affect their stability and performance. In this talk, we investigate the dissipativity of time-delay systems and derive sufficient conditions for both delay-dependent and delay-independent dissipativity. In addition, we extend the port-Hamiltonian (pH) framework to a class of nonlinear time-delay systems. We further show that delay pH systems are passive and that passivity is preserved under power-preserving interconnection. Finally, the proposed results are applied to establish the passivity of district heating networks.

**Neural Network-Enhanced Symplectic Integrators for Hamiltonian Systems**
Othmane, Amine; Flaßkamp, Kathrin
*Saarland University, Germany*
18:10

We study an approach for accelerating numerical simulations of Hamiltonian systems by combining classical symplectic integrators with symplectic neural networks. Symplectic integrators preserve the geometric structure of Hamiltonian flows but their pointwise state-prediction error is limited by numerical order and time step. Improving simulation results typically requires reducing the step size or increasing the method order, both of which increase computational cost.
We construct a corrected integrator by composing a classical symplectic method with a symplectic neural network. We show that for a fixed prediction step-size learning the correction map between the exact flow and the discrete approximation requires for desired state accuracy fewer trainable parameters than direct flow learning, with the savings increasing as the time step decreases. We analyze P-SympNets, a class of symplectic networks based on polynomial ridge functions, and establish approximation rates that relate network size to accuracy in any fixed phase-space dimension. Combined with Lie–Trotter splitting, this yields bounds on the trade-off between network capacity and approximation quality.
The learned corrector reduces local discretization error. Thus, the proposed approach permits larger time steps for a prescribed accuracy, i.e. fewer steps are required to reach a given simulation time which lowers computational cost. The composition remains symplectic, providing long-time performance. Under appropriate regularity assumptions on the Hamiltonian and with suitable architectures, we prove reductions in both local and global discretization errors over finite time intervals, leading to reduced computational time for fixed accuracy. The approach provides a mathematical framework for neural-enhanced geometric integration.

## S20.06: Modeling
Date: March 19, 2026 08:30–10:30
Room: KII, M17.17
Chair(s): Werner, Steffen W. R.
Mehrmann, Volker

**From Data To Mechanical Models Via Quadrature-based Balanced Truncation**
Werner, Steffen W. R. (1); Reiter, Sean (2)
*1: Virginia Polytechnic Institute and State University*
*2: Courant Institute School of Mathematics, Computing, and Data Science, New York University*
08:30

Learning dynamical systems from data has emerged as a pivotal area of research, bridging the realms of mathematics, engineering, and data science. Dynamical systems, which describe how states evolve over time based on underlying mathematical relations, are fundamental for understanding a wide range of time-dependent phenomena. For the use of these systems in practical applications, high modeling accuracy as well as interpretability and explainability are essential. All of these desired properties are strongly tied to the internal mathematical structure of the dynamical systems. For example,

in the modeling of mechanical or electro-mechanical processes, typically systems with second-order time derivatives occur. In this case, data are usually given in the frequency domain as samples of the corresponding transfer function. To learn such structured systems from frequency domain data, we develop in this work a data-driven second-order balanced truncation approach. This method allows the construction of low-dimensional second-order systems with generalized proportional damping structure by assembling suitable Loewner-like matrices. Numerical examples demonstrate the effectiveness of the proposed method.

**H∞model order reduction for quadratic output systems**

Hillebrecht, Birgit; Unger, Benjamin
*Karlsruhe Institute of Technology, Germany*

08:50

Systems whose outputs depend quadratically on the state arise in many areas, including port-Hamiltonian modeling, optimal control, and stochastic dynamics. In this work we study linear time-invariant systems with quadratic outputs (LQO systems) and define a suitable H∞-norm. Based on this we propose an algorithm to optimize a reduced order model with respect to this H∞norm and apply it exemplarily to the established mass–spring–damper benchmark which is modified by adding an additional quadratic output. We compare the thereby yielded models to reduced models obtained by balanced truncation and $H_2$-oriented reduction techniques.

A preprint of this work is available on arXiv: Hillebrecht, B. and Unger, B., "H∞model order reduction for quadratic output systems", arXiv e-prints, Art. no. arXiv:2505.12529, 2025. doi:10.48550/arXiv.2505.12529.

**Model reduction via adaptive domain decomposition and basis updates**

Gkimisis, Leonidas (1); Aretz, Nicole (2); Tezzele, Marco (3); Richter, Thomas (4); Benner, Peter (1,4); Willcox, Karen E. (2)
*1: Max Planck Institute for Dynamics of Complex Technical Systems, Germany*
*2: The University of Texas at Austin, USA*
*3: Emory University, USA*
*4: Otto-von-Guericke-Universität Magdeburg, Germany*

09:10

We propose a methodology for intrusive model reduction via adaptive domain decomposition. The main idea lies in adaptively segregating the computational domain into two subdomains, attributed to a reduced-order and a full-order model (ROM and FOM), respectively. Segregation is performed based on the state re-projection error at regular time intervals. Localized dynamical phenomena which do not admit an accurate low-dimensional representation via projection to the ROM basis are attributed to the FOM subdomain. Assigning a buffer zone along the ROM/FOM interface allows to dynamically capture localized phenomena, such as advection-dominated dynamics. During one adaptivity interval, a two-way coupled ROM/FOM is formulated and simulated. Subsequently, the reduced bases for both subdomains are updated by incremental singular value decomposition, so that the reduced space is enriched by the FOM subdomain simulation data. The aforementioned computational procedure enables determining the training time in an automated, space-dependent manner and encompasses an accurate model reduction solution for advection-dominated systems. We present numerical results and analyze the obtained speed-ups for two nonlinear testcases: the 1D viscous Burgers' equation and the 2D non-standard shallow-water equation.

**Optimally robust representation of (asymptotically) stable linear dynamical systems**

Beattie, Christopher (1); Mehrmann, Volker (2); Xu, Hongguo (3); Zwart, Hans (4)
*1: Virginia Tech, USA*
*2: TU Berlin, Germany*
*3: Univ. of Kansas, USA*
*4: Univ. of Twente, The Netherlands*

09:30

We present a detailed analysis of optimally robust representations for (asymptotically) stable finite and infinite dimensional linear dynamical systems. Using the solution of appropriate Lyapunov-type matrix or operator inequalities we analyze the construction of optimally robust representations.

These representations have fields of values that are bounded away from the imaginary axis in the complex left half plane and show optimal decay from a given initial value. Similar results for optimal representations of (strictly) passive dyanmical systems are also discussed.

**Map-Matching for Knowledge-Graph Based Scene Modeling in Automated Driving with a Recursive Bayes Filter and Context-Dependent Transition Dynamics**

Gerwien, Maximilian (1,2); Röbenack, Klaus (1) 09:50

*1: TU Dresden, Germany*
*2: HTWK Leipzig, Germany*

In mobile robotics and automated driving, symbolic representations with knowledge-graphs are essential for safe and interpretable planning and decision-making. We present an approach to scene modeling that solves the map-matching problem to derive the relation between dynamic objects and the road topology, as part of a knowledge-graph representation of the situation. This representation processes and abstracts sensor and map data into a formal, machine-readable model of the traffic scene, providing a robust foundation for high-level reasoning and decision-making.
In particular, the challenges and solution approaches for map-matching and the assignment of dynamic objects to a mapped road topology are discussed. Knowledge about the partially structured environment (road topology) is to be used to obtain a better estimation of the dynamic objects on the road. As a concrete solution approach, a discrete recursive Bayesian filter with context-dependent, time-varying transition dynamics is presented. With the goal is to assign noisy vehicle measurements to a known road topology represented by lanes. The discrete states are the lanes (possibly supplemented by discretized intervals) and the observations are the vehicle positions and headings, which are transformed into Frenet coordinates. The emission probability is modeled as a distribution in the lateral, longitudinal and heading direction, which models the measurement uncertainty across the lane as well as in the heading direction.
To model temporal consistency and dynamics of the vehicle movement a discrete recursive Bayes filter is applied over the lane states. The dynamic transition probability matrix is derived from the road topology and the observation horizon. It encodes possible lane transitions (e.g. lane changes, merges, splits) based on the connectivity of the lane graph within the observation horizon. This approach allows explicit modeling of temporal consistency and measurement uncertainty in map-matching, while integrating knowledge about the road topology. This approach is validated in different simulation scenarios, demonstrating its effectiveness in complex traffic situations.

## S20.07: Nonlinear control

Date: March 19, 2026 14:00–16:00
Room: KII, M17.17
Chair(s): Mironchenko, Andrii
Pauli, Patricia

**Funnel control with input filter for nonlinear systems of relative degree two**

Dennstädt, Dario; Schaa, Janina; Berger, Thomas 14:00

*Paderborn University, Germany*

We address the problem of output reference tracking for unknown nonlinear multi-input, multi-output systems with relative degree two and bounded-input bounded-state (BIBS) stable internal dynamics. We propose a novel model-free adaptive controller that ensures the evolution of the tracking error within prescribed performance funnel boundaries. By applying an output filter, the control objective is achieved without utilizing derivative information of system's output. The controller is illustrated by a numerical example.

**Stability results for interconnected PWA systems**

Cimpean, Radu; Trenn, Stephan 14:20
*University of Groningen, Netherlands, The*

In our previous work [1] we showed stability of a planar PWA system inspired by a model of the neural network responsible for detecting smells (the olfactory system). This approach was based on defining a suitable refinement of the polyhedral partition of the planar state-space and solving a corresponding set of LMIs following a method proposed in [2]. Already in [1] it was observed that extending this idea directly to a larger dimensions is, although theoretically possible, challenging and hence we proposed a decoupling approach, where the larger network is viewed as the interconnection of simple (planar) PWA systems. The coupling introduces inputs to the planar PWA which is a motivation to study input-to-state stability (ISS) of PWA systems. We will present new results about concluding global ISS from the existence of regional ISS Lyapunov functions. Furthermore, we establish LMIs whose feasibility guarantees practical ISS in each region of the polyhedral partition of the state-space.

[1] R. Cimpean and S. Trenn, "Utilizing discontinuous piecewise Lyapunov function for a biological PWA system and extending the analysis via input-to-state type stability," 2025 European Control Conference (ECC), Thessaloniki, Greece, 2025, pp. 194-200.

[2] Iervolino, R., Trenn, S., & Vasca, F. (2020). Asymptotic stability of piecewise affine systems with Filippov solutions via discontinuous piecewise Lyapunov functions. IEEE Transactions on Automatic Control, 66(4), 1513-1528

**Approximating Discrete-Time Control Barrier Function Controllers with Safety Guarantees**

Pauli, Patricia 14:40
*Eindhoven University of Technology, Netherlands, The*

Safety-critical systems in domains such as automotive engineering, robotics, and healthcare require controllers with rigorous, formally provable safety guarantees to prevent failures that could result in significant harm or damage. Control Barrier Functions (CBFs) provide a systematic framework for enforcing safety by rendering the zero-superlevel set of a CBF forward invariant while ensuring its inclusion in the safe set. While CBF-based controllers are well understood in continuous time, where the associated safety filter typically reduces to a quadratic program (QP) with a closed-form solution, the discrete-time setting lacks this favorable structure. As a result, discrete-time CBF-based controllers often involve more complex optimization problems with higher computational burden, limiting their applicability in real-time systems.

To address this challenge, we propose to approximate discrete-time CBF-based controllers using neural networks (NNs) while retaining formal safety guarantees. Our approach leverages imitation learning to replace the optimization-based control law with a learned controller that enables fast online evaluation. Specifically, we first design a robust discrete-time CBF (R-DTCBF) controller using a CBF candidate with a prescribed Lipschitz constant. We then sample the resulting control law to generate training data and train a neural network to approximate the controller. After training, we evaluate the approximation error of the learned controller. The robustness margin of the R-DTCBF explicitly accounts for approximation errors. If this error remains below the admissible bound incorporated in the R-DTCBF design, safety of the closed-loop system under the approximate controller is guaranteed. As a result, the neural network controller inherits the safety guarantees of the underlying R-DTCBF-based controller, providing a computationally efficient and provably safe alternative to optimization-based discrete-time CBF controllers.

**State Feedback Control of the Generalized Brockett Integrator**

Gerbet, Daniel; Troll, Aaron; Röbenack, Klaus 15:00
*TU Dresden, Germany*

The Brockett integrator is a third-order dynamical control system for that no everywhere continuous state feedback exists. This makes this particular system interesting for the controller synthesis and several controllers have been proposed in the past. Apart from this academic system there are

also technical systems with the same behaviour, for example non-holonomic drives or underactuated mechanical systems.

There are also some generalisations of the classical Brockett integrator. In this contribution we study one such generalisation as a dynamical system with arbitrary high state dimension, but the same structure, and show that this system can be decomposed into second-order and first-order systems by a coordinate transformation. The same transformation can be applied to the classical Brockett integrator, leading to two subsystem of dimension one and two, respectively. This transformation has some singularities, where the resulting controller is non-continuous in the original coordinates. However, the controller synthesis is thus reduced to the second-order, or the trivial first-order problem.

We discuss the controller design for the reduced problem and compose a controller for the generalized Brockett integrator from these. There is, of course, a subset of states of measure zero where the transformation is singular and a non-continuous feedback results. A choice must be made for the control at these discontinuity points.

**Criteria for input-to-output stability of infinite-dimensional systems**

Bachmann, Patrick (1); Dashkovskiy, Sergey (1); Mironchenko, Andrii (2)

*1: University of Würzburg, Germany*
*2: University of Bayreuth, Germany*

15:20

Input-to-output stability (IOS) combines the uniform global asymptotic stability of the output dynamics with its robustness with respect to external inputs. It generalizes the input-to-state stability and is a key concept for analysis and control of systems with outputs. We provide a superposition theorem for IOS of a broad class of nonlinear infinite-dimensional systems with outputs.
We introduce and analyze several novel stability and attractivity concepts for infinite-dimensional systems with outputs, such as criteria for the uniform limit property for systems with outputs, several of which are new already for systems with full-state output. Moreover, we provide superposition theorems for systems which satisfy both the output-Lagrange stability property and IOS.
Besides the challenges encountered in the classical infinite-dimensional theory, we discuss by means of counterexamples the complexities arising due to the mismatch between the dynamics of the state and of the output dynamics of the system.

**Assessing dynamical stability of data-driven surrogate models**

Grimm, Adrian (1); Mandler, Hannes (2,3); Hintz, Johanna (2); Weigand, Bernhard (3); Beck, Andrea (2); Cunis, Torbjørn (1)

*1: Institute of Flight Mechanics and Controls, University of Stuttgart, Germany*
*2: Institute of Aerodynamics and Gas Dynamics, University of Stuttgart, Germany*
*3: Institute of Aerospace Thermodynamics, University of Stuttgart, Germany*

15:40

Surrogate models are an important tool for design, maintenance, and control of technical–dynamical systems. Due to the increasing availability of real-world data, the integration of neural networks (NN) for dynamics modeling is gaining popularity. Such data-driven surrogate models (DDSM) constitute nonlinear neural feedback-loops (NFL). However, NFLs require a rigorous stability and robustness analysis as small prediction errors in the NNs accumulate in simulations of the dynamics, often leading to numerical instability. To date, the stability of NNs is often assessed on the finite training set only, which is not sufficient when the simulated inputs vary – and possibly leave the training domain – as a consequence of the simulation. There is currently no method to assess the robustness of NFLs prior to the often computationally expensive evaluation.

In this work, we utilize the systems-theoretical concept of input-to-state stability (ISS) to assess that an NFL is robust to input variations prior to its evaluation. Specifically, a system is ISS (on the operating domain), if all trajectories of the system starting within the domain will be upper bounded by a monotone function of the limiting supremum of the external input or disturbance. We show how sufficient conditions for ISS of an NFL can be verified by formulating and solving a sum-of-squares

(SOS) problem. The SOS verification can be performed before evaluation, thus avoiding the build-up of numerical errors when simulating an unstable NFL.

We demonstrate this for two applications. First, we analyze the robustness of a NN modeling the dynamics of the nonlinear Van-der-Pol oscillator as dynamic toy system. Secondly, we apply this method to DDSMs in fluid flow simulations that account for the effect of the turbulence. It was observed that DDSMs with almost perfect a priori accuracy often do not meet the high expectation towards their a posteriori accuracy of the mean flow field prediction. In fact, the simulations often become unstable. As a simple and illustrative example, we analyze a DDSM for the mixing length in a turbulent plane channel flow that is stationary in the mean, where the governing equations reduce to an ordinary differential equation in the wall-normal spatial coordinate.

## S21: Mathematical signal and image processing

Organizer(s): Berkels, Benjamin *(RWTH Aachen University)*
Effland, Alexander *(University of Bonn)*

## S21.01: Mathematical signal and image processing

Date: March 17, 2026 08:30–10:30
Room: KII, M17.16

### Optimal Transport-Based Image Processing with Applications in Watermark Recognition

Beinert, Robert 08:30
*Technische Universität Berlin, Germany*

Automated pattern recognition and classification play a central role in numerous applications and disciplines, be it in medical imaging, biometrics, or document analysis. Nowadays, in the big data regime, end-to-end deep neural networks provide the latest state of the art. In the small data regime, however, hand-crafted feature extractors and similarity measures still stand their ground. In recent years, optimal transport-based techniques like the Wasserstein distance and variations of this have become popular tools for image comparison. Although being based on a linear program, the numerical calculations of Wasserstein distances are challenging, initiating the development of linearized and sliced versions to lower the computational burden. Beyond similarity measures between images, optimal transport-based methods may be used to design feature extractors, being the focus of this talk. Ideally, a feature extractor transforms different classes to linearly separable subsets. A central inspiration behind this talk is the application of pattern recognition techniques in filigranology - the study of analogue watermarks. These play a major role in provenance research to determine the date and origin of paper-based writing and art. One of the main watermark collections is the so-called Wasserzeichen-Informationssystem (WZIS) that gathers watermarks from rubbings, hand-tracings, radiography, and thermography. Since the WZIS consists of nearly as many classes as samples, the training of common deep learning architectures does not yield reliable classifiers. Moreover, digitization techniques like the nowadays employed thermography are highly unstandardized, giving the reason to develop classifies that are invariant under affine image transformations like rotation, shifting, shearing, and scaling. Based on the one-dimensional optimal transport and the well-known Radon transform from tomography, we therefore propose flexible, easy-to-implement feature extractors that facilitate image classification tasks especially in the small data regime and guarantee linear separability of image classes that emerge from affine transformations. The proposed feature extractors are robust against non-affine image deformations, and the separability properties are provably stable provided the Wasserstein distance between the samples can be controlled. Moreover, we propose a family of generalizations to enhance flexibility and study multi-dimensional and non-Euclidean settings by making use of generalized Radon transforms. Our theoretical results are supported by numerical experiments and may pave the path towards computational filigranology.

### Accounting for model inexactness in Magnetic Particle Imaging

Nitzsche, Marius; Hahn, Bernadette 09:10
*University of Stuttgart, Germany*

Magnetic particle imaging (MPI) is a promising medical imaging technique that enables high spatial resolution and rapid data acquisition without harmful radiation.
The signal generation is based on the nonlinear magnetization response of superparamagnetic iron oxide nanoparticles, which are injected into the examined specimen and exposed to a combination of a static selection and a dynamic drive magnetic field.
The change in magnetization induces a measurable voltage in receiving coils.
The goal is then to reconstruct the spatial tracer concentration from those voltage measurements.

MPI reconstruction is highly sensitive to model inaccuracies, measurement noise, and motion during data acquisition.

In particular, the determination of the system matrix involves a trade-off between accuracy and acquisition effort, while classical reconstruction methods like regularized Kaczmarz or Landweber typically assume an accurate forward model and static tracer distributions - assumptions that are violated in practical imaging scenarios and lead to severe artefacts.

We investigate reconstruction strategies that are robust to such uncertainties without requiring explicit knowledge of their underlying sources.
The main focus is on Regularized Sequential Subspace Optimization (RESESOP), an uncertainty-aware reconstruction method that incorporates information implicitly derived from the measured data to project sequentially on suitable subspaces and to compensate for noise, model inaccuracies, and motion.

Experiments on simulated and real MPI data demonstrate significantly improved image quality, including reduced noise amplification, mitigation of artefacts caused by inaccurate system matrices, and increased robustness to motion-induced artefacts.

**Score matching meets Moreau**

Habring, Andreas; Thaler, Florian; Knoll, Thomas; Pock, Thomas
*Graz University of Technology, Austria*

09:30

In this talk we present a novel method for learning a prior for images as an energy-based model, that is, we train a functional E(x) defined on images x such that p(x) exp(-E(x)) approximates the image distribution accurately. However, instead of using, e.g., contrastive divergence or similar techniques, inspired by denoising score matching (DSM), we propose to corrupt the training data with additive Gaussian noise at different noise levels and fit p(x) so that it yields accurate reconstructions of clean images from their noisy counterparts. Contrary to DSM, instead of the MMSE denoiser, we fit the corresponding MAP denoiser to the clean image data. Via Moreau's gradient formula the training objective resembles DSM, albeit, with the gradient of the Moreau envelope of E(x) in place of the noise perturbed score. While in DSM the noise level is an additional input of the score network, this is not the case for the proposed approach since the gradient of the Moreau envelope can be computed using optimization algorithms. Therefore, the approach effectively allows us to use the information at all noise levels for training E(x) whereas in DSM a score is learned for each noise level "separately". For the proposed approach we compare two training modalities: bilevel learning and unrolling. Within the talk we motivate the training procedure, present a theoretical analysis, and show experimental results on simple toy examples as well as inverse imaging problems.

**A generalization bound for exit wave reconstruction via deep unfolding**

Atwi, Moussa; Berkels, Benjamin
*RWTH Aachen University, Germany*

09:50

Transmission Electron Microscopy enables high-resolution imaging of materials, but the resulting images are difficult to interpret directly. One way to address this is exit wave reconstruction, i.e., the recovery of the complex-valued electron wave at the specimen's exit plane from intensity-only measurements. This is an inverse problem with a nonlinear forward model. We consider a simplified forward model, making the problem equivalent to phase retrieval, and propose a discretized regularized variational formulation. To solve the resulting non-convex problem, we employ the proximal gradient algorithm (PGA) and unfold its iterations into a neural network, where each layer corresponds to one PGA step with learnable parameters. This unrolling approach, inspired by LISTA, enables improved reconstruction quality, interpretability, and implicit dictionary learning from data. We analyze the effect of parameter perturbations and show that they can accumulate exponentially with the number of layers $L$. Building on proof techniques of Behboodi et al., originally developed for LISTA, i.e., for a linear forward model, we extend the analysis to our nonlinear setting and establish generalization error bounds of order $\mathcal{O}(\sqrt{L})$. Numerical experiments support the exponential growth of parameter perturbations

**Subspace estimation from quantized samples**

Dirksen, Sjoerd (1); Li, Weilin (2); Maly, Johannes (3)
*1: Utrecht University, Netherlands*
*2: City College of New York, USA*
*3: Ludwig-Maximilians-Universität and Munich Center for Machine Learning (MCML), Germany*

10:10

We study subspace estimation from coarsely quantized data. In particular, we analyze two stochastic quantization schemes which use dithering: a one-bit quantizer combined with rectangular dither and a multi-bit quantizer with triangular dither. For each quantizer, we derive rigorous high probability bounds for the distances between the true and estimated signal subspaces. Using our analysis, we identify scenarios in which subspace estimation via triangular dithering qualitatively outperforms rectangular dithering. We verify in numerical simulations that our estimates are optimal in their dependence on the smallest non-zero eigenvalue of the target matrix, and apply them to spectral estimation.

## S21.02: Mathematical signal and image processing

Date: March 17, 2026 16:30–18:30
Room: KII, M17.16

**Adjoint mismatch in imaging problems**

Lorenz, Dirk (1); Schneppe, Felix (1); Bresch, Jonas (2); Winkler, Maximilian (1)
*1: University of Bremen, Germany*
*2: TU Berlin, Germany*

16:30

Reconstruction problems in imaging rely on a forward model and typcially a reconstruction method also needs the adjoint of the forward model (or of the derivative). In practice these adjoint methods are often implemented separately and indepently of the forward model (e.g. for fast execution). An often overlooked question is the one of adjoint mismatch: How good of an approximation is the computed adjoint for the true adjoint? In this talk we present a method that can compute adjoint mismatch between two operators, i.e. a method to compute ||A-V|| even when only evaluations of A and the adjoint of V (and not vice versa) are possible. We also comment on effects of adjoint mismatch in practice in the context of the randomized Kaczmarz method and the Chambolle-Pock method.

**Diffeomorphism-Equivariant Neural Networks**

Oettinger, Josephine Elisabeth (1); Shumaylov, Zakhar (2); Zaika, Peter (2); Lellmann, Jan (1); Schönlieb, Carola-Bibiane (2)
*1: Universität zu Lübeck, Germany*
*2: University of Cambridge, United Kingdom*

16:50

Deep learning models have become a cornerstone of modern data-driven research, yet they remain constrained by a heavy reliance on large-scale, high-quality data and intensive computational requirements. The field of Geometric Deep Learning has been established to address these inefficiencies and data constraints by incorporating group symmetries, in the form of equivariance, into neural network architectures.

In this work, we propose a strategy to transform any neural network diffeomorphism-equivariant, using an energy-based canonicalisation framework. Inspired by LieLAC, we formulate equivariance as an optimisation problem over the group of transformations, a formulation closely related to differentiable image registration. This approach achieves approximate equivariance and generalises to unseen transformations without relying on extensive data augmentation or retraining. Crucially, because the inner network remains unchanged, our framework can flexibly adapt any pre-trained network.

We provide a theoretical analysis of the framework, deriving the first non-parametric bounds on the generalisation error of energy-based canonicalisation under mild assumptions. This analysis clarifies when canonicalisation can result in good performance on previously unseen data.

The theoretical insights are reflected in DiffeoNN, a practical network architecture, which achieves approximate diffeomorphism-equivariance, illustrated on exemplary segmentation tasks. In experiments on a synthetic dataset of nested squares, DiffeoNN outperforms the naïve approach and achieves a segmentation accuracy that is comparable to a fully augmented U-Net, while requiring significantly less training data and yielding less drastic outliers. Additionally, we verify the approximate invariance of the canonicalisation step. To demonstrate applicability to large scale problems, we evaluate the performance of our network on a dataset of real-world chest X-ray images for lung segmentation, matching or outperforming the naïve approach on approximately 80% of samples.

**Trigonometric Shearlets and Where to Find Them**

Saier, Sofie 17:10
*Universität zu Lübeck, Germany*

The quality in which certain signal and image processing tasks – such as compression or edge detection – are performed depends heavily on the properties of the underlying analysis functions.

When considering local phenomena like jump discontinuities in one-dimensional data, suitable functions must themselves provide good localization. Corresponding requirements for higher-dimensional problems are more difficult to formulate (and verify), especially when local geometric properties of an edge are of interest.

Recent developments have introduced shearlet systems as powerful mathematical tools for capturing sparse directional information. However, most existing research focuses on systems defined on two- and three-dimensional Euclidean spaces. In this talk, we consider a trigonometric shearlet system on higher-dimensional tori, where methods derived from the classical fast Fourier transform enable faster computation. We generalize localization results that have proven crucial in the context of two-dimensional singularity detection [1] and, in doing so, provide insight into the construction of directionally localized polynomials on the torus.

References:

[1] Schober, K., Prestin, J., & Stasyuk, S. A. (2021). Edge detection with trigonometric polynomial shearlets. Advances in Computational Mathematics, 47(1), Article 17.

**Hilbert Transform Pairs of Wavelets**

Proell, Moritz 17:30
*University of Passau, Germany*

The orthogonal projection of a real orthonormal wavelet basis onto the Hardy space — consisting of functions whose Fourier transform is supported only on the positive real axis — yields a Parseval frame of wavelets. Motivated by practical considerations, N. Kingsbury proposed the use of two real scaling functions from multiresolution analyses (MRAs), where the corresponding wavelets form a Hilbert transform pair, to construct such a Parseval frame.
We discuss several examples of Hilbert transform pairs of wavelets: The first example, presented in the book by I. Daubechies, demonstrates that scaling functions are not uniquely determined by their scaling filter. Next, we consider a construction by I. Selesnik, which is based on an infinite product formula using sawtooth functions and a convergence criterion due to A. Cohen.
Lastly, we present a new construction of a Hilbert transform pair based on the Shannon wavelet.
We examine the properties of the resulting scaling functions and wavelets, focusing on regularity, decay, and vanishing moments.

**Analysis for Conformal Prediction Methods on Set Estimation Problems**

Jian, Xingchao 17:50
*Technical University of Munich, Germany*

Conformal prediction (CP) provides prediction sets with distribution-free guarantees. In this work we analyze CP methods for set estimation with statistically guaranteed recall rates. We focus on setCP, a non-conformity score based CP method with specific principles for score designs. We introduce two

key theoretical results: (i) setCP is equivalent to the existing conformal risk control (CRC) under mild conditions and (ii) setCP can be interpreted as imposing specific score design principles within the existing CQioC method. These findings reveal a fundamental connection between distinct CP methods. Furthermore, we provide a precise, self-contained proof of the statistical recall rate guarantee for setCP, offering additional theoretical insight into CP for set estimation beyond its links to CRC or CQioC. Statistically guaranteed solution to inverse problems can be obtained by applying CP methods on set estimation.

## S21.03: Mathematical signal and image processing

Date: March 18, 2026 08:30–09:30
Room: KII, M17.16

### Atomic Gradient Flows: Gradient flows on sparse representations

Amend, Christian (1); Zemas, Kostantinos (2); Carioni, Marcello (1) 08:30
*1: University of Twente*
*2: University of Bonn*

One of the most popular approaches for optimization problems in the space of measures are so-called Particle Gradient Flows (PGFs). For this, one restricts to linear combinations of Dirac deltas and then takes a Euclidean gradient flow in the weights and positions, significantly simplifying computations. Recent results of Chizát and Bach have shown that PGFs recover Wasserstein gradient flow dynamics, and can even converge to global minima under sufficient conditions.

In this talk, I will show an approach on how to generalize PGFs to arbitrary Banach spaces and optimization problems, which we call Atomic Gradient Flows. The crucial idea is how to choose the right notion of particles, which we argue to be extremal points of the regularizer. This extension allows, among other applications, to deal with the of BV-seminorm regularization and Optimal Transport dynamic problems.

I will discuss well-posedness and uniqueness of such Atomic Gradient Flows. Then using Choquet's theorem, I will present how to lift the problem into the Wasserstein space over extremal points and weights, discussing the relations between the lifting of the atomic gradient flow and the atomic gradient flow itself.

### Multilevel Bregman Proximal Gradient Descent

Elshiaty, Yara; Petra, Stefania 08:50
*Heidelberg University, Germany*

We present the Multilevel Bregman Proximal Gradient Descent (ML-BPGD) method, a novel multilevel optimization framework tailored to constrained convex problems with relative Lipschitz smoothness. Our approach extends the classical multilevel optimization framework (MGOPT) to Bregman-based geometries and constrained domains. We provide a rigorous analysis of ML-BPGD for multiple levels and establish well-posedness together with a global linear convergence rate. We demonstrate the effectiveness of ML-BPGD in the context of image reconstruction and validate its performance through numerical experiments.

### Multilevel Optimization on Ellipsoidal Manifolds with Applications

Vanmaele, Ferdinand-Joseph (1); Petra, Stefania (1); Stykel, Tatjana (2); Püschel, Jonas (2) 09:10
*1: Heidelberg University, Germany*
*2: University of Augsburg, Germany*

We present a Riemannian multilevel optimization framework for nonlinear optimization problems subject to ellipsoidal constraints. Such constraints naturally define Riemannian manifolds, for example weighted spheres arising from finite element discretizations or graph-based models. Our approach considers a hierarchy of discretization levels, where fine-scale models are accurate but computationally expensive, while coarse-scale models are cheaper but less detailed. To accelerate convergence on the fine level, search directions are computed using suitably constructed coarse models

that are consistent with the underlying Riemannian geometry. In particular, classical multilevel ingredients such as restriction, prolongation, and coarse corrections are generalized to manifold-valued variables, ensuring that feasibility of constraints is preserved throughout the optimization process. We illustrate the proposed framework on two nonlinear eigenvalue problems with ellipsoidal constraints: the Gross–Pitaevskii equation from quantum mechanics, and a nonlinear variant of spectral clustering arising in graph-based image segmentation.

## S21.04: Mathematical signal and image processing

Date: March 18, 2026 14:00–16:00
Room: KII, M17.16

### Generative Assignment Flows for Discrete Structured Data

Petra, Stefania 14:00
*Heidelberg University, Germany*

Measure transport and generative models constitute a major research area also in mathematical image analysis. More recently, research on generative models for discrete data which abound in scientific data analysis and mathematical imaging, has become quite active. The talk introduces a generative model for structured discrete data on graphs, which extends discriminative assignment flows for image labeling, to an approach for learning of and sampling from joint distributions of discrete random variables. The major modelling ingredients based on information geometry and Riemannian flow matching are explained and illustrated by numerical examples.

### Neural network parametrized level sets for image segmentation

Scherzer, Otmar (1,2,3); Shi, Cong (1,2); Vu, Thi Lan Nhi (1,2,3) 14:40
*1: University of Vienna, Austria*
*2: Johann Radon Institute for Computational and Applied Mathematics (RICAM)*
*3: Christian Doppler Laboratory for Mathematical Modeling and Simulation of Next Generations of Ultrasound Devices (MaMSi)*

Level set methods are a well-established approach in image segmentation, with the Chan–Vese multiphase model being a notable example. Recently, some researchers have explored parameterized versions of level set methods to enhance segmentation quality. Meanwhile, the rapid growth of neural networks in imaging has led to powerful data-driven segmentation tools. In this talk, we explore a mathematical connection between the parameterized Chan–Vese model and neural networks. The aim is to understand how classical variational models relate to neural network formulations. Specifically, we prove that a parameterized multiphase level set function corresponds to a two-layer neural network. This result provides a mathematical interpretation of certain neural network structures used in imaging tasks. Furthermore, numerical experiments are presented to demonstrate the feasibility of the proposed approach.

### Prior Knowledge-Based Analysis of Atomic Resolution Image Data

Baum, Annika; Berkels, Benjamin 15:00
*IGPM, RWTH Aachen University, Germany*

We propose a variational approach for crystal analysis based on prior knowledge.
Based on previous publications, we can already determine the repetitive motif by computing the unit cell vectors along which the image exhibits the strongest periodicity. A Gaussian bump model is used for the atom representation.
We now introduce local optimization. This adapts the atom positions within each lattice cell individually via non-linear conjugate gradient descent, seeking affine transformations that minimize the reconstruction error.
Additionally, global optimization simultaneously refines all atom positions using gradient descent on a GPU, enabling each atom to move independently.
This provides information about dislocations in the atomic pattern and can be used to detect changes

in the motif, such as twin boundaries where the motif is mirrored.
These structural boundaries are detected by computing the displacement between the original and optimized positions, applying adaptive thresholding and fitting separating tangent lines.
The method has been tested on various synthetic and experimental HAADF STEM images. The results include optimized atom positions, discrete deformation fields and automatic interface detection.

**Geometrical and statistical Mumford–Shah models for hyperspectral image segmentation**

Conrad, Fabian; Berkels, Benjamin 15:20
*RWTH Aachen, Germany*

Segmentation of hyperspectral images is challenging due to the high dimensionality, low spatial resolution, high noise, and spectral variability typically found in hyperspectral data. Since virtually no training data is available for this kind of data, we propose a fully unsupervised segmentation framework based on the multiphase Mumford–Shah model, which combines both spectral and spatial information into a single objective functional. Minimizing this objective functional then yields a segmentation.

We give a statistical interpretation of piece-wise constant Mumford–Shah models and show that the indicator functions, defining the data fidelity terms, can be chosen as negative logarithms of probability densities. We use Mahalanobis-distance-based probability densities with heavy tails to ensure robustness and to handle the high correlation between different channels. Here, we focus on the Gaussian, Student-t, and power exponential from the elliptical family as well as the log-normal distribution. This approach also enables a maximum-likelihood interpretation of the Mumford–Shah model.

Exploiting this connection between variational methods and multivariate statistics, we can improve the quality of our data fidelity term even further. The estimation of the statistical parameters is done via efficient methods for the elliptical family. Each pixel is assigned a weight that accounts for segment membership, being on a segment boundary, and being a potential outlier, which leads to more robust parameter estimates. Finally, we compare multiple indicator functions for each segment coming from multiple distributions to automatically select the indicator function that best fits the segment.

A key novelty is an edge bias that appears both in the data fidelity term and the perimeter term. In the perimeter term, it controls the relative influence on edge placement versus the data fidelity, which can be used to promote edges in flagged regions. Furthermore, the same edge bias also appears in the data fidelity term, where it downweighs pixels on the boundary of segments or mixed pixels, which are outliers from the more homogenous regions. We propose two possible, simple edge biases based on the Di Zenzo structure tensor and spectral graph theory.

We apply our segmentation framework to the standard hyperspectral benchmark datasets. After a pre-processing step using the Minimum Noise Fraction (MNF) transform, we minimize our objective functional by using a convex relaxation by Zach et al. To the best of our knowledge, the experiments show competitive to superior accuracies on all datasets compared to previous fully unsupervised methods and yield clear improvements over its Mumford–Shah-based predecessor.

## S22: Scientific computing

Organizer(s): Thomann, Andrea *(Inria Strasbourg)*
Heinlein, Alexander *(Delft University of Technology)*

## S22.01: Scientific machine learning

Date: March 17, 2026 08:30–10:30
Room: KI, M11.91
Chair(s): Heinlein, Alexander

### Differentiable PDE Solvers - A Shift of Paradigms for Numerical Simulations

Thuerey, Nils 08:30
*Technical University of Munich, Germany*

In this talk, I will talk about lessons from the area of AI / deep learning for physics simulations with numerical solvers. A key focus is the utilization of solvers that are capable of providing Jacobians, i.e. "differentiable simulations". These solvers seamlessly integrate with deep learning algorithms, presenting numerous advantages in arising from AI-based components in solvers, particularly in the context of flow simulations. However, the availability of gradient computation is not ubiquitous in many existing simulation environments. Avenues for computing them will be discussed, as well as fallbacks if they're not available (yet). I will show how to leverage differentiable solvers in varied applications such as closure modeling for Navier-Stokes, accelerated solving and inverse problems.

### Domain Decomposition and Hybridization of PINNs for scalable neural network computing

Korolev, Denis 09:10
*Weierstrass Institute, Germany*

The physics-informed neural network approach (PINNs) relies on approximating the solution to a partial differential equation using a neural network by solving an associated non-convex and highly nonlinear optimization task. Despite the challenges of such an ansatz, PINNs hold great promise for unifying various techniques into monolithic computational frameworks. In this talk, we discuss strategies for hybridizing PINNs with numerical solvers in multi-physics settings and design of stabilized PINN optimization schemes using PDE-constrained optimization. We further discuss domain decomposition approaches within the function space optimization for PINNs, laying the groundwork for scalable applications.

### Scalable Neural Network-Based Surrogate Models for Groundwater Heat Transport

Heinlein, Alexander (1); Pelzer, Julia (2); Schulte, Miriam (2); Verburg, Corné (1) 09:30
*1: Delft University of Technology, Netherlands, The*
*2: University of Stuttgart, Germany*

Machine learning methods often struggle in real-world scientific and engineering applications due to limited or low-quality training data and complex physical dependencies. We consider the example of groundwater flow with heat transport, which can be modeled as an advection-diffusion process under heterogeneous flow conditions with spatially varying material parameters and distributed heat sources. Classical numerical simulations of such scenarios are computationally demanding due to high spatio-temporal resolution requirements and large domain sizes.

While purely data-driven surrogate models can be more efficient, they often fail to accurately predict advection-dominated processes, which are highly sensitive to input variations and exhibit long-range spatial interactions. To address these challenges, we introduce a surrogate modeling approach that combines a lightweight numerical surrogate for the global transport process with convolutional neural networks to model local groundwater velocity and heat diffusion effects.

Using the proposed framework, we model city-scale subsurface temperature fields with heterogeneous groundwater flow and up to one hundred groundwater heat pump injection points, resulting in interacting thermal plumes over long distances. The approach is first systematically analyzed using

randomized subsurface parameter fields. Subsequently, the model is trained on a small number of cut-outs from a real-world subsurface parameter map of the Munich region and is shown to generalize to significantly larger domains without retraining.

**Machine Learning Surrogate Modeling for Homogenization of Hyperelastic Materials with Boolean Microstructures**

Brändel, Matthias; Rheinbach, Oliver 09:50
*Technische Universität Bergakademie Freiberg, Germany*

Data-driven surrogate models offer an efficient alternative to repeated numerical homogenization of heterogeneous materials. In this contribution, a supervised learning approach is presented for predicting effective parameters of hyperelastic composites from low-dimensional microstructural descriptors. The training data is based on previously published numerical homogenization results for ensembles of two-phase stochastic microstructures generated by planar Boolean models, covering variations in inclusion shape, phase contrast, and area fraction, see Brändel, Brands, Maike, Rheinbach, Schröder, Schwarz and Stoyan (2022). A neural network is trained to map area fraction, specific surface, and material parameter ratios to effective Neo-Hookean parameters. Additional datasets representing limiting cases of the parameter space are incorporated to stabilize training and improve extrapolation behavior. Numerical results demonstrate that the network trained on these descriptors predicts effective material parameters with sufficient accuracy for a range of microstructures. At the same time, systematic deviations between different inclusion shapes suggest that the incorporation of higher-order geometric features could further improve predictive performance.

**Finite Operator Learning with Neural-Initialized Newton Solvers**

Taghikhani, Kianoosh (1); Najian Asl, Reza (2); Apel, Markus (1); Rezaei, Shahed (1) 10:10
*1: Access e.V. Aachen, Germany*
*2: Technical University of Munich, München, Germany*

Neural operators have recently emerged as a powerful framework for learning mappings between function spaces, making them well suited for solving partial differential equations governing complex physical systems.

We discuss how classical numerical methods, particularly the finite element method (FEM), can be embedded into neural operators to make them physics informed and, at the same time, how classical solvers can be extended through parametric learning. Within this unified framework, we investigate several architectures, including Fourier Neural Operators (FNO), DeepONet, and conditional neural fields as a more general modeling platform for spatiotemporal and pseudo-static mechanical problems in heterogeneous materials. We further introduce a Finite Operator Learning formulation in which the discretized weak form of the underlying energy functional is embedded directly into the loss function. This construction does not rely on automatic differentiation, and boundary conditions are enforced in a hard manner. The formulation leads to improved learning of both primal variables and their gradient fields.

In addition to the above ideas, we propose a Neural-Initialized Newton (NiN) strategy, in which neural operator predictions are used to initialize Newton–Raphson solvers. This initialization significantly improves robustness and convergence, enabling convergence within a single load increment and reducing the number of Newton iterations by up to an order of magnitude for highly nonlinear problems.

**S22.02: Research software engineering**
Date: March 17, 2026 16:30–18:30
Room: KI, M11.91

**What is an RSE, and what is the community doing?**

Thiele, Jan Philipp
*TU Braunschweig, Germany*

16:30

The term Research Software Engineering was coined over ten years ago.

Since then, many people have identified as RSEs and gathered in communities and associations, like de-RSE e.V. in Germany or the new GAMM activity group RSE & RDM.

As the goal of sustainable research software aligns well with the need for reliable and reproducible scientific computing, we want to give an overview of the developments and activities around the term RSE. More specifically, we give a more concrete definition of what an RSE is, e.g. based on competencies, and present some current projects like the curriculum for a Master in RSE or the conceptualization of a German research software institution.

**MathModDB: A Database for Mathematical Models**

Fiedler, Jochen (1); Biedinger, Christine (1); Reidelbach, Marco (2); Schembera, Björn (3); Schmidt, Burkhard (4); Shehu, Aurela (4); Koprucki, Thomas (4)
*1: Fraunhofer Institut für Techno- und Wirtschaftsmathematik*
*2: Zuse Institut Berlin*
*3: Universität Stuttgart*
*4: Weierstraß-Institut für Angewandte Analysis und Stochastik*

16:50

The systematic documentation, discovery, and reuse of mathematical models — especially across disciplines — is a challenging problem. In this contribution, we introduce the database MathModDB, an ontology and knowledge graph for mathematical models. MathModDB provides a semantic description of mathematical models for the discovery of existing, alternative, competing, or complementary models within and across disciplines. Developed within the Mathematical Research Data Initiative (MaRDI) of the Nationale Forschungsdateninfrastruktur (NFDI), MathModDB supports and enhances the search for information on models and related literature, conducted by researchers beyond a classical keyword search. Thus, MathModDB implements the FAIR principles (Findable, Accessible, Interoperable, Reusable) for mathematical models and makes them also machine-readable and machine-actionable, ready for integration into scientific computing tools chains, workflow systems (e.g. Snakemake) and other domain-specific knowledge graphs (e.g. Plasma KG).

MathModDB defines a data model with classes, object properties/relations, data and annotation properties as an ontology, basically consisting of the classes Mathematical Model, Mathematical Expression, Computational Task, Quantity, Quantity Kind, and Scholarly Article, with many links to external ontologies such as QUDT (Quantities, Units, Data Types) or knowledge graphs such as Wikidata. Currently, the MathModDB database holds 20.000 statements on more than 200 models. These include use cases from computational mechanics (cooperation with NFDI4Ing and Bundesanstalt für Materialforschung, Berlin) and plasma physics (cooperation with Leibniz Institute for Plasma Science and Technology, Greifswald).

The current implementation of MathModDB is embedded in the MaRDI Portal, a web-service and infrastructure built upon the WikiBase technology stack to access the MaRDI Knowledge Graph, which also comprises a huge number of publications, authors, software packages, and data sets. Moreover, MathModDB is closely intertwined with MathAlgoDB, a database of mathematical algorithms, also developed within MaRDI. Both databases are directly connected to MaRDMO, a mathematics-specific extension of the Research Data Management Organiser (RDMO) which represents a convenient way to populate the knowledge graphs. The combination of MaRDMO with MathModDB and MathAlgoDB enables researchers to document mathematical models, numerical algorithms, and computational workflows in a structured way.

Future work will focus on community-drivencontributions and curation, as well as integration with workflow systems such as the NFDI4Ing Model Validation Platform. We invite researchers to explore MathModDB at https://portal.mardi4nfdi.de/wiki/MathModDB or directly at the MaRDI exhibition booth during the GAMM conference.

**Extensible data and algorithm dispatch for flexible benchmarking in applied mathematics and mechanics**

Saak, Jens; Nayak, Ashwin S.; Benner, Peter 17:30
*Max Planck Institute for Dynamics of Complex Technical Systems, Germany*

Benchmarking numerical algorithms on curated examples against community-accepted measures such as runtime and accuracy is crucial in computational workflows. It is necessary that these benchmarks are reproducible and transparent to enrich the scientific output, and several NFDI consortia aim to provide the necessary infrastructure to carry these out in their respective domains. MaRDIMark is the benchmarking framework developed by MaRDI, the mathematical NFDI consortium.

The benchmarking process is segmented into five distinct modules within the MaRDIMark benchmark framework. Examples and algorithms are the initial two modules representing the data and algorithms under investigation and their combination and relationship, collectively define a problem. The remaining three components denote sequential stages during actual benchmark runs: driver, analyzer and explorer. The driver stage performs the actual execution of algorithms solving a list of problems and storing their solutions along with time measurements, potential estimates of the energy consumption from hardware counters, or internal estimates of the mathematical measures of interest (e.g., residual or error norms). In the second stage, the analyzer module investigates the solutions applying a selection of measures, e.g., explicit computation of error norms or residual norms, or validating expected mathematical properties of the solutions. Lastly, the explorer provides users the ability to compile reports of their quantities of interest from the results of the previous stages. These reports can take various forms, such as text, tables, or figures and be stored in various output formats, depending on the desired use case.

From an abstract perspective, examples, solutions, and benchmark results are just different types of structured data. Meanwhile, the algorithms to be tested, measures to be taken, as well as report generators are algorithms applied on these structured data. The relationships between mathematical objects and algorithms play a crucial role in the orchestration of a benchmark run, and knowledge graphs such as MathAlgoDB and MathModDB can provide the necessary structure to formally represent and organize this interplay. In this contribution, we demonstrate how object-oriented software design patterns, such as factories, can be used to dispatch data and algorithms based on knowledge-graph queries, and thus make benchmark tools easily extensible.

**MaRDMO: FAIR Documentation of In-Silico Research**

Reidelbach, Marco 17:50
*Zuse Institute Berlin, Germany*

Scientific computing brings together mathematical modeling, numerical algorithms, software, and data to enable in-silico experiments for the solution of complex real-world problems. While methodological progress is essential, the long-term impact of computational research increasingly depends on how these heterogeneous components are documented, connected, and made reusable across projects and disciplines. In practice, however, models, algorithms, and interdisciplinary workflows are still rarely described in a structured and interoperable way.
This contribution presents MaRDMO as a domain-specific extension of the Research Data Management Organiser (RDMO) that places the needs of scientific computing at the center of research data management. MaRDMO provides tailored questionnaires and automated interfaces to different knowledge bases, enabling researchers to document mathematical models, algorithms, and interdisciplinary workflows as coherent computational resources rather than isolated artifacts.
Through direct integration with services of the Mathematical Research Data Initiative (MaRDI) such

as the Mathematical Model Database (MathModDB), the Mathematical Algorithm Database (MathAlgoDB), and the MaRDI Portal, as well as external sources like Wikidata, MaRDMO supports the standardized description of key elements of in-silico experiments from model assumptions and mathematical formulations to numerical methods, software implementations, and interdisciplinary workflow structures. Automated metadata pre-filling reduces manual effort and helps embed FAIR principles directly into everyday scientific computing practice.
MaRDMO can be deployed within existing institutional RDMO installations at universities and research centers, allowing it to integrate seamlessly into established data management support structures. In addition, the MaRDI RDMO instance, provided through the NFDI basic service DMP4NFDI, offers a ready-to-use access point for researchers without local RDMO infrastructure, further lowering the threshold for adoption. Completed documentations can be directly published and shared with the community via the MaRDI Portal, turning local documentation into reusable research objects for scientific computing.
By strengthening the infrastructure layer that connects modeling, computation, and application, MaRDMO supports reproducibility, interdisciplinary transfer, and the sustainable use of mathematical methods in application-driven research and makes structured research data management an integral part of modern in-silico research.

**Software package MaRDI Open Interfaces for increased interoperability in computational science**

Kabanov, Dmitry; Rave, Stephan; Ohlberger, Mario
*University of Münster, Germany*
18:10

MaRDI Open Interfaces is a software package that aims to help scientists conduct computational experiments that involve numerical solvers written in different languages and having diverse programming interfaces.
To this end, the software decouples scientists' computational code from the details of a concrete solver through generic interfaces for typical numerical problems, such as optimization or time integration, and automatic cross-language data-type conversions.
Hence, the software package provides computational scientists flexibility in switching solvers written by different research groups and potentially implementing different numerical algorithms for the same problem type or avoid writing bindings (when none are provided) to these solvers, saving time on code modifications and testing.
In our talk, we show how to use the software package as well as that the performance overhead remains negligible, especially in the light of the provided flexibility.
This work is a part of the Germany-wide project Mathematical Research Data Initiative (MaRDI) of the National Research Data Infrastructure (Nationale Forschungsdateninfrastruktur, NFDI).

## S22.03: Computational fluid dynamics

Date: March 18, 2026 14:00–16:00
Room: KI, M11.91
Chair(s): Thomann, Andrea

**A simple and general framework for the construction of exactly div-rot-grad compatible discontinuous Galerkin finite element schemes on unstructured simplex meshes**

Dumbser, Michael
*University of Trento, Italy*
14:00

We introduce a new family of discontinuous Galerkin (DG) finite element schemes for the discretization of first order systems of hyperbolic partial differential equations (PDE) on unstructured simplex meshes in two and three space dimensions that respect the two basic vector calculus identities exactly also at the discrete level, namely that the curl of the gradient is zero and that the divergence of the curl is zero. The key ingredient is the construction of two compatible discrete nabla operators. An important feature of our new method is the fact that only two different discrete function spaces are needed

to represent the numerical solution, and the choice of the appropriate function space for each variable is related to the origin and nature of the underlying PDE. The first class of variables is discretized at the aid of a *discontinuous* Galerkin approach, where the numerical solution is represented via piecewise polynomials of degree N and which are allowed to jump across element interfaces. This set of variables is related to those PDE which are mere consequences of the definitions derived from some abstract scalar and vector potentials. The second class of variables is discretized via classical *continuous* Lagrange finite elements of approximation degree M=N+1 and is related to those PDE which can be derived as the Euler-Lagrange equations of an underlying variational principle. The primary nabla operator takes as input the data from the FEM space and returns data in the DG space, while the dual nabla operator takes as input the data from the DG space and produces output in the FEM space. The two discrete nabla operators satisfy a discrete Schwarz theorem on the symmetry of discrete second derivatives. From there, both discrete vector calculus identities follow automatically. We apply our new family of schemes to three hyperbolic systems with involutions: the system of linear acoustics, the vacuum Maxwell equations and the Maxwell-GLM system of Munz et al., which contains a unique mixture of curl-curl and div-grad operators and in which the magnetic field may be either curl-free or divergence-free, depending on the choice of the initial data. In all cases we prove that the proposed schemes are exactly total energy conservative and thus nonlinearly stable in the L2 norm.

**An Entropy Stable Discontinuous Galerkin Spectral Element Method on Heterogeneous Grids**

Keim, Jens; Schwarz, Anna; Kopper, Patrick; Rohde, Christian; Beck, Andrea 14:40
*University of Stuttgart, Germany*

The discontinuous Galerkin spectral element method (DGSEM) has proven to be a highly efficient numerical scheme for the approximation of smooth multiscale problems, e.g., turbulence in the present case. Key aspects for the high efficiency are its excellent parallelization properties and the use of a tensor-product ansatz, where the multidimensional space operator is decomposed into a sequence of
one-dimensional operations. Efficient and robust application-oriented large eddy simulations (LES) of turbulence were enabled by the use of entropy-stable DGSEM in a flux differencing formulation. In its classical tensor-product formulation, the entropy stable DGSEM was first only developed for quadrilateral and hexahedral elements. However, for the discretization of complex geometries, more flexible
element types, e.g., simplexes, are in general more favorable. In a recent work, Montoya and Zingg presented an efficient entropy stable flux differencing DGSEM formulation on triangular and tetrahedral elements. To benefit from the computational efficiency of the tensor-product ansatz, the authors used a collapsed coordinate transformation on Legendre–Gauss-Lobatto and Legendre-Gauss-Radau nodes. The authors were able to show that their scheme is computationally more efficient as previously developed entropy stable schemes which utilize a full-order basis. Moreover, the intrinsic drawback of small time steps in the collapsed coordinates formulation was resolved by the temporal evolution of modal degrees of freedom (DOFs) instead of nodal ones.
In practical applications such as the flow around an airfoil in the majority of the computational domain, the use of, e.g., hexahedral elements can be favorable and only in a small subset, e.g., simplexes are required. For this, the approach of Montoya and Zingg is extended to triangular prism, pyramid and tetrahedral elements on Legendre–Gauss nodes to enable an efficient entropy stable DGSEM on heterogeneous grids. To avoid any load imbalances due to the additional modal switching of the residual on non-hexahedral elements, a time measurements based partitioning technique is employed for the load balancing.
In the present talk, an entropy stable DGSE scheme on heterogeneous meshes is presented. A particular focus is placed on the collapsed coordinates transformation, the interelement flux computation between different elements types, the modal time-update of the non-hexahedral elements, and the load balancing strategy. The free-stream preservation and the convergence properties are demonstrated based on numerical experiments and the excellent scaling properties of the DGSEM are shown. The talk concludes with application-oriented numerical problems.

**Energy stability and conservation properties of the Domain of Dependence stabilization on two dimensional cut cell meshes**

Birke, Gunnar (1); Engwer, Christian (1); May, Sandra (2); Petri, Louis (3); Ranocha, Hendrik (3) 15:00

*1: University of Münster, Germany*
*2: Technical University of Berlin*
*3: University of Mainz*

Cartesian cut cell meshes are constructed by embedding object boundaries in a structured cartesian mesh and removing the intersection between objects and cartesian cells, leading to so called cut cells. This gives an easy and efficient procedure to discretize complex geometries at the cost of potentially having very small cells in the mesh, putting severe restrictions on the time step size when explicit Runge-Kutta schemes are employed.
The Domain of Dependence stabilization method consists of penalty terms on top of a standard discontinous Galerkin scheme enabling a time step size based on the cartesian structured mesh by establishing information flow directly between neighbors of small cells, preventing overshoots on these small cells.
We present an abstract framework for the DoD stabilization based on a splitting of numerical fluxes into central and dissipative parts which is provable energy stable (or even conservative) for linear equations. As a numerical test example we consider the acoustic wave equation. We will also discuss some numerical results for the Euler equations.

**A data-driven approach to cut-cell quadrature using spline interpolation**

Mika, Michał (1); Hiemstra, Rene R. (2); Stoter, Stein K. F. (2); Schillinger, Dominik (1) 15:20

*1: Technical University of Darmstadt, Germany*
*2: Eindhoven University of Technology, The Netherlands*

We present a data-driven approach to develop higher-order accurate tensor-product stencil quadrature rules for implicitly defined two-dimensional domains. We construct a three-dimensional configuration space of possible domain cuts using a signed distance representation based on circular arcs, defined by their radius and center, and exploit symmetry to simplify its three-dimensional domain. The configuration space, being piecewise smooth, is carefully partitioned into smooth regions, enabling three-dimensional tensor-product spline interpolation to approximate quadrature data sampled from an established implicit domain quadrature technique. The resulting quadrature rules are simple to apply, highly accurate, efficient, and can be used as a black-box solution. We demonstrate compatibility with existing cut finite element techniques and illustrate their application through numerical examples.

**Lattice Boltzmann Method for solids: high-performance 3D elastodynamics solver using NVIDIA Warp**

Weverbergh, Julie (1); Boolakee, Oliver (1); Geier, Martin (2); De Lorenzis, Laura (1) 15:40

*1: ETH Zurich, Switzerland*
*2: TU Braunschweig, Germany*

The Lattice Boltzmann Method (LBM) has recently been developed to solve problems in solid mechanics, starting with linear elastostatics and continuing with linear elastodynamics in two dimensions. Based on these works, we propose an extension of LBM for linear elastodynamics in three dimensions. Using the asymptotic expansion technique, we prove second-order consistency for periodic, Dirichlet and Neumann boundary conditions for 3D prismatic domains. The scheme is stable under a CFL-like condition. Numerical experiments are conducted to verify our theoretical derivations. Furthermore, we assess the computational performance on a GPU architecture using XLB, an accelerated Lattice Boltzmann library based on the NVIDIA Warp backend. We demonstrate that the

proposed LBM approach enables faster simulations than a conventional explicit FEM scheme when applied to large-problem sizes.

## S22.04: Linear solvers

Date: March 18, 2026 16:30–18:30
Room: KI, M11.91
Chair(s): Heinlein, Alexander

### Extrapolated Multigrid Methods for Elliptic PDEs on Non-Polygonal Domains

Dasari, Sai Aakash (1); Kruse, Carola (1); Mycek, Paul (1); Rüde, Ulrich (2) 16:30
*1: CERFACS*
*2: FAU Erlangen-Nürnberg*

Extrapolated multigrid methods use coarse-grid information to improve both the accuracy of the discrete solution (differential convergence) and the efficiency of the solution process (algebraic convergence). For elliptic finite element systems on polygonal domains, this approach is equivalent to a defect-correction multigrid scheme with a higher-order discretization when using specific quadrature rules.

We extend this methodology to domains with curved boundaries, such as the cross-sections of tokamak reactors. Initial numerical experiments using extrapolation with linear finite elements on a non-nested grid hierarchy show accuracies of the same order as quadratic isoparametric elements.

This approach avoids the implementation difficulties of optimized higher-order isoparametric finite element codes while preserving multigrid efficiency and providing improved solutions on non-polygonal domains.

### Smoothed Aggregation Algebraic Multigrid for Problems with Heterogeneous and Anisotropic Material Behavior

Firmbach, Max (1); Phillips, Malachi (2); Glusa, Christian (2); Popp, Alexander (1); Siefert, Christopher M. (2); Mayr, Matthias (1) 16:50
*1: University of the Bundeswehr Munich, Germany*
*2: Sandia National Laboratories, USA*

Many modern engineering applications - such as thermal diffusion, groundwater flow, and electrostatics - involve materials with heterogeneous and often highly anisotropic properties. Numerical simulations of such systems are challenging, as finite element discretizations tend to produce poorly scaled and ill-conditioned linear systems. To ensure efficiency and scalability, iterative solvers preconditioned with algebraic multigrid (AMG) methods are widely employed. However, conventional AMG techniques typically do not account for material heterogeneity or anisotropy, resulting in slow convergence or even failure. Although recent progress has been made for mesh-induced anisotropy, the robust treatment of genuinely heterogeneous and anisotropic materials remains an open problem.
In this talk, we present a new smoothed-aggregation strategy that incorporates material information directly into the AMG coarsening process. In contrast to classical strength-of-connection heuristics, which often perform poorly in the presence of coefficient jumps and directional anisotropy, the proposed approach is robust, easy to apply, and effective across a wide range of scenarios. In particular, for problems with strongly directional material behavior, we demonstrate that the iteration counts become independent of the material contrast. We also discuss the implications of Jacobi-based prolongation smoothing for ill-conditioned fine-level operators and introduce a matrix-filtering procedure based on a targeted dropping scheme. This filtering controls operator complexity throughout the multigrid hierarchy, ensuring that the computational cost of the preconditioner remains low.

**Identification of Performance-Critical Solver Parameters in Multilevel Block Preconditioners for Multiphysics Systems**

Bühler, Regina (1); Brandstaeter, Sebastian (1); Popp, Alexander (1); Mayr, Matthias (1,2) 17:10

*1: Institute for Mathematics and Computer-Based Simulation, University of the Bundeswehr Munich, Germany*
*2: Data Science & Computing Lab, University of the Bundeswehr Munich, Germany*

Monolithic approaches for coupled multiphysics systems usually yield large, sparse, block-structured linear systems whose solution often dominates the overall simulation time. Achieving robust and scalable performance typically requires multilevel block preconditioners with many algorithmic parameters. In practice, these parameters are often tuned based on expert experience or limited trial-and-error studies, which becomes infeasible in high-dimensional parameter spaces. This work addresses the problem of identifying performance-critical solver parameters, taking time-to-solution as the performance metric. Such insight is essential to reduce computational cost on high-performance computing systems while preserving robustness of the underlying algorithms.

Therefore, we propose to apply variance-based global sensitivity analysis (GSA) to algebraic multigrid preconditioning for block-structured systems. State-of-the-art studies typically report iteration counts or timings for a few hand-picked configurations and thus provide only local information. In contrast, we explore a broad region of the parameter space and quantify the global influence of each parameter on solver performance via Sobol indices [1]. To make this feasible for computationally expensive multiphysics simulations, we construct a surrogate performance model based on Gaussian process regression, trained on a moderate number of solver runs and evaluated cheaply for Monte Carlo estimation of Sobol indices. This combination of GSA and surrogate modelling yields a mathematically grounded ranking of solver parameters and identifies parameters with significant impact on performance.

This presentation focuses on the proposed methodology, from constructing the surrogate-based performance model and designing the GSA study to computing and interpreting Sobol indices for representative multiphysics benchmarks. We illustrate the approach with numerical experiments on coupled problems such as fluid-structure interaction [2] or contact mechanics [3]. The results show how the Sobol indices determine a subset of performance-critical parameters and identify others as negligible, thereby reducing the dimension of the tuning problem. This presentation provides insight into a systematic, transferable methodology for analysing parameter influence in preconditioned iterative solvers for multiphysics applications.

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**Multilevel Monolithic Overlapping Schwarz and Geometric Multigrid**

Köhler, Stephan; Rheinbach, Oliver 17:30

*Technische Universität Bergakademie Freiberg, Germany*

Domain decomposition methods of the additive overlapping Schwarz type provide iterative approaches for solving partial differential equations.
The incorporation of coarse levels enables these methods to achieve both numerical and parallel scalability.
Among successful coarse space strategies, the generalized Dryja–Smith–Widlund (GDSW) space,

drawing inspiration from iterative substructuring techniques, has proven particularly effective.
Building on the GDSW framework, Heinlein, Hochmuth, Klawonn (2019) developed two-level monolithic overlapping Schwarz preconditioners specifically designed for saddle point problems.
This contribution presents parallel computational results for incompressible fluid flow problems, combining geometric multigrid algorithms and a (multilevel) monolithic overlapping Schwarz preconditioner for the coarse problem of the the multigrid algorithm.
The presented results leverage the synergy between the Fast and Robust Overlapping Schwarz (FROSch) library—integrated within the ShyLU package of Trilinos—and the FEATFLOW library, interconnected through a scalable interface that ensures efficient coupling between both software frameworks.
This work is part of the StroemungsRaum project, financed by the German BMFTR (formerly BMBF) under the SCALEXA program, the German initiative to develop software in the exascale computing era.

**Accelerating Matrix Inversions using Random Butterfly Transformations and Local Pivoting**
Köhler, Martin (1); Sievers, Julian (2) 17:50
*1: MPI Magdeburg, Germany*
*2: OvGU Magdeburg, Germany*

Computing the matrix inverse is a procedure that is rarely used in scientific computing. One notable exception is Newton iteration for computing the matrix sign function, sign(A). Typically, the matrix inverse is computed by employing the partial pivoted LU decomposition (GEPP), followed by triangular inversion; or via the Gauss-Jordan elimination (GJE) with partial pivoting. In both cases, partial pivoting introduces two issues with regard to current computer architectures. Firstly, the pivoting procedure itself is a bottleneck on multi-core CPUs and GPUs, as it introduces additional synchronization points, thereby reducing the parallel structures in the LU decomposition. Secondly, pivoting causes many non-local data accesses and movements are caused, resulting in many inefficient memory transactions. To avoid this, the current approach is to use the Random Butterfly Transform (RBT) and the LU decomposition without pivoting (GENP). Together with iterative refinement, this approach is effective for linear systems $Ax = b$ with a small number of right-hand sides. However, when applied to computing the matrix inverse, this procedure requires more than twice the floating-point operations of the GEPP-based approach. In our contribution, we demonstrate how iterative refinement in the inversion process can be avoided. To achieve this, we combine the RBT approach for LU decomposition with a local pivoting strategy. This enables the use of parallelization strategies known for non-pivoted LU decomposition, but with increased accuracy. Furthermore, we extend this approach to Gauss-Jordan elimination. Integrating the new procedure into the computation of the matrix sign function of size 40,960 results in a speedup of 3.89 compared to classical partial pivoted LU decomposition, and is 1.86 times faster than using the Gauss-Jordan elimination procedure. Finally, we demonstrate how this integrates in the Matrix Sign Function based solvers for the Sylvester and Lyapunov equation.

**An Example of Linear Systems on a Neuro-Inspired Platform**
Gebert, Johannes (1); Bouslama, Amir (2); Stockmann, Lukas (1); Widmayer, Sven (1) 18:10
*1: High-Performance Computing Center Stuttgart, Institute for High-Performance Computing, University of Stuttgart, Germany*
*2: Technical University of Munich, Chair of Computational Mathematics*

Physical scaling limits lead to stagnating performance gains for von Neumann machines, usually based on host CPUs and GPUs for acceleration. However, the scientific community still strives for another thousandfold increase in computational performance, achievable through lower-precision arithmetic in the early 2030s. We expect that emerging hardware paradigms, in particular neuro-inspired computers, will help build computers that deliver an additional leap in performance at reasonable cost and with relatively low energy consumption.
Neuro-inspired computing paradigms will not succeed if there is no readily available stack of compilers, libraries, performance analytics, and other tooling to enable their practical use. Furthermore, they must support existing applications due to the cost and effort required to develop and maintain

them.
With NeuroFEM, Theilmann and Aimone demonstrated that hardware-implemented neuronal networks can solve sparse-matrix linear systems. Consequently, we assume that applications relying on those linear systems, e.g., finite element methods (FEM) and computational fluid dynamics, can compute their computationally intensive mathematical kernels on neuro-inspired hardware. Proving this general viability for computing ideally relies on a relevant, well-understood simulation with available source code.
In this conference paper, we evaluate the use of our biomechanical FEM software, Direct Tensor Computation (DTC), which implements direct numerical simulations of structural mechanics using computed tomography (CT) scans to calculate patient-specific effective stiffness parameters. We cover the entire pipeline for reading a CT image, solving the linear system, and postprocessing. Furthermore, we define the solution of the verified and validated Fortran implementation as the ground truth.
SpiNNaker 2 is a general-purpose, neuro-inspired platform. We ported DTC to Python without replicating its massively parallel features or the data structures from its Fortran origin. We convert the linear system from its sparse-matrix form to the sparse neural network format required by the SpiNNaker platform and solve the linear systems using firing neurons.
One-to-one comparisons need to be taken with a grain of salt, due to significant differences between von Neumann and neuro-inspired hardware architectures. Nevertheless, comparisons of the Fortran-based ground truth and the neuro-inspired solution are insightful for the general viability, memory use, performance, and numerical precision.
Overall, we present the current state of solving sparse linear systems for scientific applications on neuro-inspired hardware. We conclude with further research and collaboration opportunities.

## S22.05: Meshing, finite element methods and applications

Date: March 19, 2026 08:30–10:30
Room: KI, M11.91
Chair(s): Thiele, Jan Philipp

### A Generic Discrete Space-Filling Curve for Scalable Adaptive Mesh Refinement

Dreyer, Lukas (1); Holke, Johannes (2)
*1: Leibniz Universität Hannover, Germany*
*2: German Aerospace Center (DLR)*
08:30

Adaptive mesh refinement is a central technique in scientific computing, enabling accurate simulations at manageable computational cost. Large-scale AMR frameworks, however, often suffer from complex and duplicated code bases, particularly in the implementation of space-filling curves, which play a crucial role in mesh traversal and data management in forest-of-trees methods.
We present a new abstract formulation of a discrete space-filling curve designed for forest-of-trees meshes. The core idea is a template-based, dimension-independent design that unifies all element types within a single implementation. This removes the need for separate curve variants for triangles, quadrilaterals, tetrahedra, hexahedra, and hybrid meshes. Integrated into the open-source AMR library t8code, the new formulation reduces the code size related to space-filling curves by a factor of more than four, significantly improving maintainability and extensibility. The generality of the formulation also opens a path toward supporting higher-dimensional mesh topologies, including potential future applications to 4D meshes arising in spacetime simulations.
In addition to this structural simplification, the redesigned curve yields about 5–10% performance improvement in core traversal and indexing routines. The abstract structure leads to more effective compiler optimization by reducing branching and improving inlining opportunities. These local speedups carry over to higher-level AMR operations while preserving the communication behavior and partition stability of the previous implementation.
We further summarize benchmark studies evaluating the scalability of t8code's main algorithms, including refinement, coarsening, partitioning, and ghost-layer construction, and show that the new curve integrates efficiently into large-scale parallel workflows.
Finally, we highlight ongoing work coupling t8code with the finite-element library deal.II, where the

simplified curve design supports scalable adaptive simulations across a wide range of application areas.

**hp-Quadrature for One-Loop Feynman Integrals in the LTD Framework**

Dölz, Jürgen (1); Duhr, Claude (2); Kovačić, Bartul (1); Semper, Cathrin (2) 08:50
*1: Institute for Numerical Simulation, University of Bonn*
*2: Bethe Center for Theoretical Physics, University of Bonn*

Making precise perturbative predictions for collider experiments, such as those at the Large Hadron Collider (LHC), requires evaluating highly complex multi-loop Feynman integrals in physical kinematic regions. Alongside analytical methods, numerical techniques are increasingly important, but many of them rely on Monte Carlo algorithms and therefore suffer from slow convergence. Once a solid understanding of the singularity structure of these integrals is obtained and divergences are properly regulated, our goal is to tackle this challenge using an hp-quadrature approach.
Using a novel Loop-Tree Duality (LTD) technique, one can rewrite Feynman integrals as integrals over Euclidean space. The resulting integrands can be expressed as a sum of limits of functions that converge to functions singular on multiple convex manifolds and their intersections. By exploiting the convexity of these manifolds, it is possible, for simpler geometries, to analytically decompose the integration domains. This decomposition allows the use of hp-quadrature methods to achieve high-precision results, with errors that decrease exponentially with the quadrature order. This talk will present the formulation of the problem for one-loop integrals, highlight the challenges of this approach, and discuss representative numerical results.

**Fast static condensation: A linearly scaling operator for non-constant diffusivities**

Huismann, Immo 09:10
*DLR e.V., Germany*

This paper derives a decomposition of the static consensed element operator for a spectral-element method for the Poisson equation for non-constant diffusivities.
It allows to evaluate the static condensed element operator in $O(n^3)$ operations per element, where n is the number of points per hexahedral element, i.e. scaling linearly with the number of degrees of freedom in the full mesh.
Numerical tests prove the exactness of the operator by comparing to the full operator, and runtime measurements demonstrate the linear scaling.

**Experimental and Numerical Investigation of Jump Phenomena in the Frequency Response of Piezoelectric Systems**

Friesen, Olga; Hölscher, Jonas; Siegmund, Michael B. K.; Claes, Leander; Henning, Bernd 09:30
*Measurement Engineering Group, Paderborn University, Germany*

Piezoelectric ceramics are used in a wide range of fields, including high-power ultrasound applications such as ultrasonic bonding. The behaviour of these components in resonance excitation shows pronounced nonlinear properties. In practice, these nonlinear effects lead to a number of phenomena, including voltage-dependent resonance shifts and a characteristic tilting of resonance curves. These phenomena have a significant impact on the performance, stability and control of the components but cannot be described by linear models. Consequently, the accurate prediction of the behaviour of resonances in piezoelectric components remains a significant challenge when operating at resonance with elevated excitation voltages.

In this contribution, an experimental and numerical study on the nonlinear resonance behaviour of piezoceramic rings is presented. An experimental setup is developed to measure electrical properties for both increasing and decreasing frequency sweeps under varying excitation voltages. For this purpose, a network analyser with a suitable power amplifier is used. The observed outcome includes distortions of the frequency response, a pronounced tilting of resonance curves, and jump phenomenon. These observations serve as a basis for the development and validation of nonlinear material models.

For the numerical analysis, the piezoelectric constitutive relations are extended by a polynomial nonlinear stress-strain relationship to account for field-dependent material behaviour. In order to fit the simulated responses to the experimentally measured resonance characteristics a suitable parametrisation of the nonlinear terms is chosen. Since the excitations are assumed to be harmonic, a harmonic balancing finite element method approach is used assuming axial symmetry. Due to this simplified nonlinearity model and the usage of the harmonic balancing method, the simulations can be performed efficiently. A comparison between simulation and experiment demonstrates a reasonable degree of agreement for the resonance under investigation and for a range of excitation voltages. The results provide insight into the suitability and limitations of polynomial nonlinear material models for resonant piezoelectric systems.

**Partial Observation of Linear Systems with Mori-Zwanzig Formalism**

Wang, Fan (1,2); Benner, Peter (1); Heiland, Jan (3)

*1: Max Planck Institute for Dynamics of Complex Technical Systems, Germany*
*2: Department of Mathematics, Otto-von-Guericke-University Magdeburg*
*3: Department of Mathematics and Natural Sciences, Ilmenau University of Technology*

09:50

Model order reduction (MOR) aims to reduce the computational cost of complex dynamical systems while preserving the behavior of important variables. Most existing MOR methods assume that a full-order model (FOM) is available. However, in many applications—such as molecular dynamics and climate systems—the FOM is unknown, and only partial observations or data streams can be accessed.
The Mori–Zwanzig (MZ) formalism [2, 3] provides an exact reduced description for systems with partial observations by using a projection-operator framework. This equation consists of three parts: (1) a Markovian term describing instantaneous effects, (2) a memory term that accounts for the influence of unresolved variables through time history, and (3) a stochastic forcing term representing remaining unresolved effects.
In our work, we derive the MZ reduced dynamics for partially observed linear systems and construct a computable representation of the memory kernel. We then present numerical experiments for both ODEs and PDEs with partial observations. The results show that the MZ framework can accurately predict the evolution of observed variables even when a large part of the system is unobserved.
Finally, we explain the connection between empirical model reduction (EMR) [1] and the MZ formalism. EMR can be interpreted as a data-driven closure of the MZ equation, where the memory term is approximated by a finite number of variables, leading to a Markovian representation. In this setting, the fitted stochastic forcing corresponds to the noise term generated by the MZ orthogonal dynamics. This viewpoint unifies projection-based and data-driven model reduction methods and provides a practical approach for reduced modeling when the full-order model is inaccessible.

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**Novel Algorithms for Nonlinear Root-Finding: Perpendicular and Extended Secant Methods with CADNA Implementation**

Miah, Md. Asadujjaman (1); Noeiaghdam, Samad (2); Hossan, Md. Shorif (3) 10:10
*1: Department of Applied Mathematics, University of Dhaka, Dhaka, Bangladesh.*
*2: Institute of Mathematics, Henan Academy of Sciences, Zhengzhou 450046, China.*
*3: Department of Statistics and Data Science, Southern Methodist University, Dallas, Texas, USA.*

A fundamental challenge in computational mathematics is the reliable and efficient computation of roots of nonlinear equations. This paper presents and investigates two new derivative-free techniques: the **Perpendicular Method (PM)** and the **Extended Secant Method (ESM)**. The PM enhances the classical regula falsi scheme through a geometric perpendicular-line construction that improves approximation accuracy, while the ESM generalizes the conventional secant formula via an nnn-power modification that delivers superlinear convergence approaching the golden ratio. Both methods are described through clear iterative algorithms and illustrated with corresponding flowcharts to emphasize their computational structure. The paper establishes convergence results for each method through formal theorems, and integrates the **CESTAC** (Contrôle et Estimation Stochastique des Arrondis de Calculs)stochastic arithmetic strategy, implemented in the **CADNA** (Control of Accuracy and Debugging for Numerical Applications) library, to monitor rounding-error propagation, detect numerical instabilities, and determine optimal iteration stopping points. The main CESTAC theorem is employed to validate accuracy and ensure self-verified computations. Numerical experiments on several nonlinear benchmark problems demonstrate that ESM consistently converges faster than classical Newton, secant, bisection, and regula falsi methods, whereas PM provides higher precision compared to regula falsi. Overall, combining PM and ESM with CESTAC significantly improves robustness by addressing intrinsic, branching, and cancellation instabilities while providing reliable, automatically validated approximations.

## S22.06: Scientific computing in applications

Date: March 19, 2026 14:00–16:00
Room: KI, M11.91
Chair(s): Thomann, Andrea

**A Flexible Open-Source Finite Element Platform for Redox Flow Battery Modeling**

Aghabarari, Amirhossein (1); Horsch, Martin Thomas (1); Janssen, Mathijs (1); Valseth, Eirik (1,2); Dokken, Jørgen S (2) 14:00
*1: Norwegian University of Life Sciences, Norway*
*2: Simula Research Laboratory, Norway*

Redox flow batteries are one of the promising options for large-scale, long-term energy storage. In this work, we consider vanadium redox flow batteries (VRFBs). The performance of VRFBs is governed by the coupled effects of transport and electrochemical phenomena. Industrial simulators are often costly and operate as non-transparent black boxes. This has motivated the development of several free battery simulation tools, such as PyBaMM, BattMo, and EZBattery.

In this work, we aim to develop an open-source and flexible finite element-based simulation environment for VRFB half-cells. As a starting point, we consider a VRFB half-cell as a representative redox flow battery configuration. For this half-cell, we develop a macrohomogeneous finite element model implemented in the open-source FEniCS framework, and compare its performance with widely used open-source tools in the battery-modeling community, such as PyBaMM, as well as other simulators reported in the literature. The electrochemical model is formulated using a homogenized porous electrode description with effective transport properties, charge conservation in the solid and electrolyte phases, and Butler–Volmer kinetics. We study discretizations with different numbers of elements and orders of approximation in various spatial dimensions.

We extensively verify and validate our developed model by first considering simplified benchmark problems. In these benchmarks, our finite element discretization exhibits faster and more systematic convergence to reference solutions than the alternative tools considered. After verification and

validation against the benchmark problems, we extend the half-cell model by adding additional physical effects, including multiple vanadium species, contributions from migration to ion transport, and velocity distributions in the electrolyte domain. We show that the improved accuracy and convergence properties carry over to these more realistic cases. We demonstrate that our finite element model for simulating redox flow batteries matches the predictions of reference open-source battery solvers at the half-cell level, while offering superior flexibility and scalability for complex geometries and multiphysics extensions. The resulting workflow provides an open-source modeling framework for half-cell redox flow batteries that can be extended to full-cell and stack-scale analyses.

**Efficient Numerical Simulation of Excitonic Drift–Diffusion Models for Organic Photovoltaics**

Çiloğlu, Pelin (1); Tretmans, Carmen (2); Pietschmann, Jan-F. (2); Stoll, Martin (1) 14:20

*1: University of Technology Chemnitz, Germany*
*2: University of Augsburg, Germany*

We present a numerical framework for analyzing the device performance of organic solar cells by coupling the drift–diffusion equations with an exciton kinetics model. The approach incorporates complex morphological information obtained from previously computed phase-field simulations of bulk-heterojunction structures. These morphologies, which encode the spatial distribution of polymer, non-fullerene acceptor, and interfacial regions, are directly embedded into the drift–diffusion system to provide spatially varying, physically realistic material parameters.
To solve the coupled nonlinear system, we employ three numerical schemes, Newton, Gummel, and Semi-Newton–Gummel, together with a finite-element discretization and robust linear solvers. The method accurately captures the interplay between exciton generation, diffusion, dissociation, and the transport of charge carriers under applied voltage. Numerical experiments demonstrate the impact of morphology on the resulting current–voltage characteristics and validate the effectiveness of the proposed computational approach.

**Model adjustments and solver construction for galvanic cells based on NPP-systems**

Schwöbel, Stephan; Mehner, Thomas; Lampke, Thomas 14:40

*TU Chemnitz, Germany*

Electroplated coatings on metallic substrates have a wide range of practical applications ranging from corrosion or wear protection on parts, good conductivity on electrical contacts to coating systems for bipolar plates in fuel cells. Modelling and simulation are extremely important for achieving efficiency and effectiveness in both the coating and use of components. The large field of applications in electrochemical engineering motivates several questions for scientific computation, such as the simulation of coating thickness distributions and alloy-composition distributions on the cathode leading to nonlinearly coupled PDEs with nonlinear boundary conditions. Although in recent years many advances have been made in the scientific computation of electrochemical systems for electroplating, important questions are still open. These include the integration of large reaction systems into the models and their numerical treatment as they have a major impact on the electroplating process and the resulting layer. The given contribution addresses the modelling of reactions in the galvanic cell as well as electrode reactions specifically and constructs a suitable methodology to simulate the modelled system to obtain reliable and meaningful simulation results. In particular, the talk addresses convenient strategies to decouple and simplify the resulting large system of PDEs for efficient and comparingly fast simulations.

**Spatiotemporal Reaction–Diffusion Modeling of Wolbachia Persistence in Aedes aegypti Populations**

Mena, Hermann (1); Benner, Peter (1); Ramirez, Carmen (2); Rodriguez, Jarvy (2) 15:00

*1: MPI Magdeburg, Germany*
*2: Universidad del Valle, Cali, Colombia*

We present a comprehensive spatiotemporal model to investigate the invasion, spread, and long-term persistence of *Wolbachia* infections in *Aedes aegypti* mosquito populations following the release

of infected carriers. The model is formulated as a system that couples biologically informed reaction–diffusion processes with mechanisms of imperfect vertical transmission, spatial heterogeneity, and mosquito movement. The analytical framework exploits mathematical tools from dynamical systems, spatial ecology, and partial differential equations to characterize invasion thresholds, stability conditions, and qualitative behavior across parameter regimes. By integrating ecological features and strain-specific biological parameters, our framework enables a comparative analysis of distinct *Wolbachia* strains, highlighting how differences in transmission efficiency and fitness effects shape spatial spread and persistence. We combine analytical insights with systematic numerical simulations to discuss relevant questions: (i) the influence of release size and spatial distribution on establishment success, (ii) strain-dependent conditions that maximize long-term persistence, and (iii) the interplay between environmental heterogeneity and infection dynamics over extended time horizons. Given the global burden of mosquito-borne diseases, particularly dengue, our results might provide enough quantitative guidance for designing sustainable biological control strategies, bridging mathematical theory with applied public health objectives. The proposed model contributes to a deeper mathematical understanding of spatially structured biological invasions and supports evidence-based decision-making in vector control programs.

**Efficient Numerical Methods for the Simulation of Post-Pumping Saltwater Intrusion Experiments**

Nägel, Arne 15:20
*Goethe University Frankfurt, Germany*

Salinization of coastal aquifers is a current problem in many regions worldwide and simulation of this process is an important tool for the forecast of drinking water resources. When fresh water producing wells are present, density effects play an important role. In this case, a high degree of accuracy is required for both the position of the phreatic (unsaturated) zone and the freshwater interface.

We present a model for haline density-driven flow problem in partially saturated aquifers, which is based on a generalized Richards equation. Nonlinear effects and the large temporal and spatial scales of the aquifers, pose a challenge for the solution of the coupled system of PDEs. In the suggested approach, the system is discretized using a finite volume method method and an adaptive linearly implicit time-stepping scheme. The resulting linear systems are then solved using a multigrid method. The implementation is based on the UG4 software toolbox and the related parallel groundwater flow simulator d3f++. The high-performance computing (HPC) potential of the overall approach is assessed and demonstrated in numerical experiments.

Moreover, the model is successfully used to describe the dynamics of the post-pumping seawater intrusion experiment of Stoeckl et al, which tracks the inland migration of the saltwater interface after pumping cessation. The uncertainty in the key hydrogeological parameters is addressed by a reduced order model, that is based on a Hierarchical Tucker (HT) tensor representation. This allows to describe 10 million parameter-dependent time series by only several thousand fully computed simulations. The reduced order model is used to investigate parameter-dependent variability and to identify combinations that best match the experimental observations.

**Bayesian inference for bathymetry reconstruction**

Stietz, Lars (1,2); Götschel, Sebastian (1); Ruprecht, Daniel (1); Schleper, Peter (2) 15:40
*1: Hamburg University of Technology, Germany*
*2: University of Hamburg, Germany*

Inverse problems appear in all scientific domains. Approaches to solve inverse problems can be put into two categories, minimizing an objective function using suitable regularization techniques to deal with the inherent ill-posedness, or formulating the inverse problem in a statistical sense and approximating the posterior distribution for the parameters of interest. The inverse problem we consider in this talk is the reconstruction of the bottom topography of rivers, lakes or oceans, also called bathymetry, from measurements of the water height. Knowledge about the bathymetry is important for maritime science and civil engineering, as well as shipping operations and flood management.

We reconstruct the bathymetry in a wave flume from real-world measurements. Shallow water equations are used to describe the flow and water level in the experiment. For the statistical approach we employ Bayesian inference for the bathymetry reconstruction. In particular, we use a Markov chain Monte Carlo method, to obtain estimates as well as uncertainties for the parameters of interest from the posterior distribution. We discuss the choice of prior distributions, and compare the results of the Bayesian inference with an adjoint optimization approach.

## S23: Applied operator theory

Organizer(s): Post, Olaf *(Universität Trier)*
Schlichting, André *(Universität Ulm)*

## S23.01: Applied operator theory

Date: March 19, 2026 08:30–10:30
Room: KII, M17.99
Chair(s): Post, Olaf
Schlichting, André

### Continuum limit of Lipschitz learning on sparse graphs

Roith, Tim (1); Bungert, Leon (2); Calder, Jeff (3)
*1: Deutsches Elektronen-Synchrotron DESY, Germany*
*2: University of Würzburg*
*3: University of Minnesota*

08:30

This talk is devoted to proving continuum limits of Lipschitz Learning. Given a partial labeling on a finite data set, the goal is to extend the labels to the whole data set without increasing their Lipschitz constant. We are interested in the continuum limit of this problem when the number of data points tends to infinity. This is first done via $\Gamma$-convergence of the graph Lipschitz constant functional to the functional $u \mapsto ||\nabla u||_\infty$. The corresponding minimization problem is a Lipschitz extension task, which does not admit a unique solution. We then consider absolutely minimizing Lipschitz extensions (AMLEs) which are the unique solution of the infinity Laplace equation. We show that convergence rates of graph to continuum AMLEs can be derived from a ratio convergence property of distance functions. This is then applied to arbitrary geometric graphs as well as to homogeneous Poisson point processes. In both cases, our techniques yield convergence rates for very sparsely connected graphs.

### Mean-field approximation for particle interaction on adaptive networks

Throm, Sebastian
*Umea University, Sweden*

08:50

We consider interacting particle systems with an underlying adaptive network structure, i.e. both the particles and the network evolve in time with coupled dynamics. We study the infinite particle limit for a large class of network-particle interactions and provide corresponding limit descriptions of the coupled system.

### On the spectrum of positivity-preserving mass transport on graphs

Stephan, Artur
*Technische Universität Wien, Austria*

09:10

We consider the linear evolution of mass transport on a graph described by a drift on the edges and a coupling in the nodes. From the functional analytic side, the process is modeled by Markov generators of positive semigroups either on the space of continuous functions (backward equation) or the space of probability measures (forward equation). The framework naturally accommodates positive mass distributions on both edges and nodes.
In the talk, we present a general structure of boundary conditions that satisfies positivity and mass conservation. In addition, we derive the stationary measure, and, in the corresponding $L^2$ space, we analyze the dissipativity arising from the boundary conditions. Interestingly, it turns out that there is no energy-dissipation inequality of Poincaré type. However, by investigating the spectral function directly, one can estimate the spectrum and find examples that either possess or lack a spectral gap. The talk is based on a joint work with Holger Stephan (Berlin).

**On homogenisation of linear nonlocal problems in fractional divergence form**

Buchinger, Andreas (1); Burazin, Krešimir (2); Crnjac, Ivana (2); Erceg, Marko (3); Jolić, Maja (2); Waurick, Marcus (4)

*1: TU Hamburg, Germany*
*2: School of Applied Mathematics and Informatics, University of Osijek, Croatia*
*3: Faculty of Science, University of Zagreb, Croatia*
*4: TU Bergakademie Freiberg, Germany*

09:30

In this work, we are interested in linear nonlocal problems in fractional divergence form with highly oscillatory coefficients. Here, the notions of fractional gradient and divergence follow the theory of Riesz fractional gradients (cf. Shieh and Spector (2015)). Recently, Caponi et al. (2025) introduced a variant of *H*-convergence for the coefficients of these problems and proved the corresponding compactness.

In this talk, we build upon these results to provide a characterisation of this newly established notion of *H*-convergence. We achieve this by means of classical *H*-convergence, which captures the local behaviour of the fractional divergence form problem, and $L^\infty$-weak* convergence on the complement, arising from the nonlocality of the differential operators. Finally, we describe these results in the light of nonlocal *H*-convergence as introduced by Waurick (2018) and discuss their connection to certain Schur topologies.

**Well-posedness and passivity for a class of bilinear systems**

Dahmani, Abdelhakim (1); Gernandt, Hannes (1,2); Hosfeld, René (3); Reis, Timo (4); Tasci, Tolgahan (1); El Haskouki, Ikram (1)

*1: University of Wuppertal*
*2: Fraunhofer IEG*
*3: TU Berlin*
*4: TU Ilmenau*

09:50

Bilinear systems generalize linear control systems by allowing the input operator to depend linearly on the state. Such bilinear systems yield a broad class of models that arise in diverse applications, including quantum control, district heating networks, and mechanical systems such as beams with controlled damping.

In this talk, we present a general framework for bilinear systems on Banach spaces and establish existence and uniqueness of classical solutions by extending known results for mild solutions under suitable admissibility conditions on the input operators. Moreover, in the Hilbert space setting, we prove passivity of the bilinear systems under additional dissipativity assumptions on the generating semigroup.

The theoretical results are illustrated through applications to a bilinear Schrödinger equation, a district heating network and a bilinear controlled Fokker-Planck equation.

**On Rayleigh scattering in massless Nelson models**

Kußmaul, Valentin; Griesemer, Marcel

*Universität Stuttgart, Germany*

10:10

It is an open problem to establish asymptotic completeness (AC) of Rayleigh scattering in models of atoms interacting with quantized radiation. The obstacle is the lack of a sufficient control on the number of emitted photons. Assuming a bound, uniform in time, on the expected number of emitted photons, there is a proof of AC by Faupin and Sigal. We simplify that proof, and most importantly we replace the assumed bound by a weaker assumption concerning the decay of the distribution of the number operator for large times. Our assumption is both necessary and sufficient for AC.

## S24: History of applied mathematics and mechanics

Organizer(s): Wagner, Jörg *(University of Stuttgart)*
Ceranski, Beate *(Universität Stuttgart)*

### S24.01: History of Applied Mathematics and Mechanics: Players

Date: March 19, 2026 08:30–10:30
Room: KII, M17.73
Chair(s): Ceranski, Beate
Wagner, Jörg

#### The Members of GAMM 1922-1933

Lemberg, Jason 08:30
*University of Wuppertal, Germany*

There is not much research on the formation of GAMM. The existing literature provides an overview of the institutionalization of GAMM with two dominant interpretations: On the one hand Helmut Gericke points to professional reasons, whereas Renate Tobies on the other hand stresses connections to the economy and the military. This difference is remarkable. In my presentation I will argue that both authors are correct by looking at the GAMM membership.

To gain a more nuanced understanding of GAMM's early history, the membership of GAMM in the Weimar Republic will be examined using membership lists. This goes beyond the description of GAMM's leading committees provided in the literature so far. The aim is a topography of early Applied Mathematics and Mechanics. A quantitative overview of the number of members and their nationality is provided and the following questions are addressed: What was the affiliation of GAMM members? Which academic status groups did they belong to? What was their professional specialization? What were their connections to the economy and the military?

This is to bridge the seemingly contradictory interpretations found in the literature and improve our understanding of the early history of GAMM.

#### Die Geschichte der Vorgängerorganisationen des Deutschen Zentrums für Luft- und Raumfahrt e. V. (1907-1945): Ein Schulterblick in ein aktuelles Forschungsprogramm

Wichner, Jessika; Beckmann, Daniel; Wucherpfennig, Jens 09:10
*Deutsches Zentrum für Luft- und Raumfahrt e. V., Germany*

Das Deutsche Zentrum für Luft- und Raumfahrt (DLR) hat 2023 eine vierjährige wissenschaftliche Aufarbeitung der Geschichte seiner Vorgängerorganisationen in der ersten Hälfte des 20. Jahrhunderts gestartet.

In insgesamt acht Projekten wird die Geschichte der Vorgängerorganisationen des DLR im Zeitraum 1907 bis 1945 durch renommierte Historikerinnen und Historiker untersucht. Neben dem Schwerpunkt auf die Zeit des Nationalsozialismus werden auch der Erste Weltkrieg und die Zeit der Weimarer Republik analysiert.

Im Rahmen der Projektlaufzeit werden fünf geschichtswissenschaftliche Monografien, zwei Bildbände sowie eine Wanderausstellung und ein dazugehöriger Ausstellungskatalog entstehen, die sich an unterschiedliche Zielgruppen richten. Ein zentraler Aspekt wird die Frage der Darstellung der wissenschaftlichen Ergebnisse gegenüber der Öffentlichkeit sein.

Um eine externe Qualitätssicherung zu garantieren und sicherzustellen, dass die Historikerinnen und Historiker ihre Projekte in freier Forschung ohne Intervention des Auftraggebers durchführen können, begleitet ein interdisziplinär besetzter Beirat die Aufarbeitungsaktivitäten. Dieser berät sowohl die Projektbearbeiterinnen und Projektbearbeiter als auch die mit der organisatorischen Durchführung des Forschungsprogramms betrauten Mitarbeiterinnen und Mitarbeiter des DLR.

Der Vortrag gibt einen Schulterblick in das Aufarbeitungsprogramm. Dabei wird unter anderem erläutert, wie die Historikerinnen und Historiker für die Projektarbeit gewonnen wurden, wie die Vernetzung der Forscherinnen und Forscher über die Projektstudien hinweg gelang, und wie die Zusammenarbeit mit dem Beirat erfolgt.

Ferner werden die thematischen Schwerpunkte der einzelnen Projekte aufgezeigt und flankierende Aktivitäten vorgestellt, die ergänzend zur Arbeit der Historikerinnen und Historiker durchgeführt werden. Dazu zählt zum Beispiel ein Dokumentarfilm, der die Vorgängerorganisationen des DLR in dem zu untersuchenden Zeitraum in den Blick nimmt.

Begleitet werden die Aufarbeitungsaktivitäten von einer Agentur, welche die Aufgabe hat, die finalen Produkte ansprechend und einheitlich zu gestalten. Auch diese Zusammenarbeit wird thematisiert werden.

Der Vortrag wird nicht die wissenschaftlichen Ergebnisse der Studien präsentieren. Diese werden zu gegebener Zeit unter Einbeziehung der Historikerinnen und Historiker vorgestellt.

**The Curious Life of Walter Lode**

Bruhns, Otto T. 09:30
*Ruhr University Bochum, Germany*

Walter Lode was born on January 5, 1898, in Mühlhausen (then province of Saxony/Prussia) as the son of the textile wholesaler Paul Lode and his wife Minna Lode, née Mehler.

When World War I broke out, he was student at the local high school. Despite excellent grades in mathematics and natural sciences, he left school with his father's permission in September 1914 to join the German army as a war volunteer at the age of 16. At the end of the war, he was discharged as lieutenant in Göttingen, near his hometown. At this time, Germany was in a state of unclear political situation and ongoing unrest. Thus, he joined the Göttingen vigilantes in 1919 and took part in the suppression of the Ruhr uprising in March and April 1920 as a member of a volunteer corps. From the beginning of 1919, he studied physics and mathematics at the Georg August University in Göttingen. As one of the lesser known students of the Göttingen School, he completed his doctorate in 1926 at the Institute for Applied Mechanics of Ludwig Prandtl and under the supervision of Árpad Nádai with a thesis on the influence of the intermediate principal stress on the yielding of metals.

After having completed his doctorate and further experimental work for Nádai, in 1928 he joined Bayer AG in Elberfeld. He worked as a physicist at this company for over three decades, most recently as head of the mathematics group in the applied physics engineering department. During this time, he worked in medical research, later, he was heavily involved in the area of rubber research and development. This, incidentally, protected him during World War II from being sent to the front again. He reported on this work only after the war during a stay in Manchester in 1947/1948. Much of his work was reflected in corresponding patents. Even after his retirement, he published papers, mainly in the field of standardization and its application. At the age of 83, he died on March 15, 1979, in Leverkusen.

**Beam bending: Was Leonardo right?**

Kienzler, Reinhold 09:50
*University of Bremen, Germany*

Leonardo da Vinci (1452-1519) is well-known for his paintings and sculptures, also for his inventions in the fields of architecture, civil and mechanical engineering. He is less known for his contributions in solid mechanics. Despite quite philosophical reflections on the notion of force and other phenomena, he treated beam bending intensively.

In this contribution, I intend to show to what extent Leonardo had an idea of the correct theory of beam bending.

## S24.02: History of Applied Mathematics and Mechanics: Methods and Objects

Date: March 19, 2026 14:00–16:00
Room: KII, M17.73
Chair(s): Wagner, Jörg
Ceranski, Beate

### Exciting objects for historical research – Mechanical gyroscopes in Germany between 1925 and 1975

Niklaus, Maria (1,2) 14:00
*1: Verkehrsmuseum Dresden, Germany*
*2: University of Stuttgart, Germany*

The contribution presents a dissertation project in the history of science and technology that uses gyro instruments as objects of historical research, offering exciting opportunities for investigation using a wide variety of methodological approaches. As material sources, they reveal the maturation and closing of technology and its impact on the actors and institutions associated with it. The focus is here on mechanical gyroscopes between ca. 1925 and 1975 in Germany: First as direct display devices in aircraft cockpits and, in another example, as parts of automatic control systems.

Not only long lines of continuity in technology can be found but also at the expert and user levels. In addition to researching the habitus of communities in professional societies and through objects, invisible hands, here in research and manufacturing, can also be made visible again through object research approaches.

Objects are also used by gyro experts to place their own achievements outside the community. The example of a controversy can be used to clarify many of the methods used and clearly demonstrate the attempt to highlight one's own achievements, i.e. to make these invisible objects in a museum visible again.

Further attention is paid to users of these instruments. For various user groups, gyro instruments disappear as mature technology in several stages after it had led to fears of being replaced by machines. This can be seen in different application contexts. However, due to discontinuities, gyro instruments can then only become partially visible again.

Overall, this work is a plea for the investigation of (gyro) instruments after the successful use of objects as historical sources.

### A historical mechanical construction as a possible foundation of artificial intelligence, with a dynamical systems perspective

Gunesch, Roland 14:20
*Pädagogische Hochschule Vorarlberg, Austria*

This talk presents a mechanical construction which was created as a thought experiment and which was historically one of the early attempts to create a physical model for cognition, the Braitenberg vehicles. Although they are a very simple physical construction, they already exhibit surprisingly complex behaviour which is similar to cognitive activity which is usually associated with either complex biological organisms or with much larger constructions (computational machines) that simulate biological cognition.

This is especially interesting now in the age of dramatically increasing powers of artificial intelligence, because the current/modern approach to creating artificial intelligence typically uses huge amounts of input data and large amounts of computing power. In contrast to that, the Braitenberg vehicles are extremely simple analog systems. This simplicity is useful even in modern settings.

When viewing Braitenberg vehicles from the point of view of the theory of dynamical systems, an interesting mathematical theory can be developed.

Although this is a historical approach (and, by the standards of the theory of artificial intelligence, old), the topic is still of current research interest, particularly in areas such as neuroscience and robotics.

**The development of rheology as a science**

Altenbach, Holm 14:40
*Otto-von-Guericke-Universität Magdeburg, Germany*

The first rhelogical investigations were performed may be in the ancient Egypt. A significant step forward was achieved with the work of Hooke, Newton, and other contemporaries: the first laws of rheology were formulated. Over the next 200 years, further special rheological equations were suggested so that experimental observations could be described more accurately. However, only the discussions and collaboration of E.C. Bingham and M. Reiner result in establishment of the science of rheology in the 20s of the last century.

The contibution is focussed on some historical remarks, the basics of rheology in the sense of Bingham and Reiner, and, finally, on some recent developments in this field.

**The long shadow of Karl Weierstraß over the calculus of variations**

Ullrich, Peter 15:00
*Universität Koblenz, Germany*

At first glance, Karl Weierstraß's (1815–1897) contributions to the calculus of variations were only published in the seventh volume of his *Gesammelte Werke* [Weierstraß 1927], thirty years after his death. However, the content of his lecture courses on the calculus of variations had already influenced the presentations of other mathematicians on this topic, who also paid him due recognition, such as Adolf Kneser (1862–1930) in [Kneser 1900] and Oskar Bolza (1857–1942) in [Bolza 1904] and [Bolza 1909].

Of particular importance in this context is the lecture course from the summer semester of 1879, in which Weierstraß introduced his field concept for the calculus of variations and which has already been analyzed by Rüdiger Thiele [Thiele 2007]. In addition, Weierstraß expressed his views on the calculus of variations in his letters to Hermann Amandus Schwarz (1843–1921), for example on the relationship between the variation of functions and the variation of curves, as well as his plans for a book on the calculus of variations.

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**Caring about the Material Culture of Mathematics and Mechanics: Collections and Networks at the University of Stuttgart**

Ceranski, Beate
*Universität Stuttgart, Germany*

15:20

In the last decades the material culture of science, especially in the form of university collections, has received increasing attention. In contrast to the neighbouring classical universities the University of Stuttgart has no central curator. Yet it disposes of a rich landscape of collections and dedicated local curators. Coming together in the *Sammlungsnetzwerk* (network of collections), the local curators – substantially supported by the university library – have developed many and multifaceted activities from brochures to exhibitions and 3D digitalization of objects.

The talk will give both an overview and specific examples for objects, collections and activities in some pertinent subjects and disciplines such as mathematical models and instruments, the computer museum (with a collection of calculating machines) and the important collection of gyroscopes.

Finally the talk will also adress the question why science departments and universities should care about their material heritage. At a technically oriented institution such as the University of Stuttgart, whose identity is informed by the everlasting quest for cutting-edge technological solutions, this represents a highly nontrivial issue.

The talk also serves as an introduction to the visits to some collections that will be offered later in the afternoon.

## S25: Machine Learning and Data Science in Applied Mathematics and Mechanics

Organizer(s): Stoll, Martin *(TU Chemnitz)*
Fritzen, Felix *(Universität Stuttgart)*

## S25.01: Mathematics of Machine Learning

Date: March 17, 2026 08:30–10:30
Room: KII, M17.01
Chair(s): Stoll, Martin

### Data analysis of architected structural geometries with persistent homology

Milor, Abel (1); Salvalaglio, Marco (1,2)
*1: Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany*
*2: Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany*

08:30

Designing novel materials with superior and resilient mechanical properties requires precise tailoring of their structures. In particular, the design of architected metamaterials, which feature carefully engineered geometries, represents a promising path given their versatility. Their structural arrangements are typically highly complex, characterized by nontrivial and often disordered configurations. Despite this complexity, their geometries must be represented in a numerically tractable manner to enable practical applications in data-driven materials science. Consequently, identifying suitable morphological descriptors for data analysis and algorithmic modeling, in particular for computing suitable inputs to machine learning models, presents a significant challenge. In this context, novel methods from applied topology emerge as powerful tools to address this challenge. Among them, persistent homology enables extracting and representing local geometrical features as point clouds, effectively converting complex structural information into simple data. This transformation facilitates the application of data science techniques, including statistical analysis and machine learning models, to gain deeper insights into material structures. Here, we discuss the application of persistent homology to characterize correlated disordered structures. Focusing on the case of Gaussian Random Fields, we show that persistent homology efficiently describes structural properties that only appear on large scales, such as hyperuniformity. We further illustrate that this description is exploitable for inferring nontrivial structural characteristics of patterns in a data-driven fashion, compatible with machine learning models. Finally, we explore promising extensions of this framework regarding its applicability to the mechanical engineering of metamaterials. This includes structures such as spinodoid architectures, where topological analysis can provide valuable insights into their design and performance.

### Does Double Descent Resolve the Accuracy-Complexity Trade-Off in the Offline Training of Data-Driven Turbulence Closure Models?

Mandler, Hannes (1,2); Grimm, Adrian (3); Cunis, Torbjörn (3); Beck, Andrea (2); Weigand, Bernhard (1)
*1: Institute of Aerospace Thermodynamics, University of Stuttgart, Germany*
*2: Institute of Aerodynamics and Gas Dynamics, University of Stuttgart, Germany*
*3: Institute of Flight Mechanics and Controls University, University of Stuttgart, Germany*

08:50

Due to the ever-increasing need for more accurate turbulence closure models, the growing amount of publicly available direct numerical simulation (DNS) data and the popularity of machine learning methods, recalibrating existing closures and tailoring them for particular applications has become an active research field. Most commonly, the closure coefficients are modeled by a neural network (NN) that was trained on DNS data to predict the optimal values of the coefficient based on mean flow quantities.
As this offline recalibration process does not take the dynamic interaction of the NN with its injection environment (the flow solver) into account, a target conflict between maximizing the NN's accuracy

and minimizing its complexity arises. On the one hand, one may expect the highest accuracy gains if the NN describes the training data well and is therefore tempted to maximize the NN's size. This yields complex NNs and may ultimately lead to overfitting.
On the other hand, the ill-conditioning of the RANS equations may cause an exponential growth of initially tiny errors over the course of the simulation. An upper bound for the error growth rate can be obtained using the NN's Lipschitz constant (LC). If the NN fits the data well, it is likely to have a large LC potentially causing strong error accumulation in the flow solver. If the NN's LC is limited during its training, though, the potential for improvement in the mean flow field prediction by introducing the NN into the closure model decreases.
However, recent results from deep learning show that the generalization error of NNs may not necessarily increase as the NNs grow. In fact, NNs seem to use additional degrees of freedom that they do not need to memorize the training samples to smoothen their predictions in-between the training samples. This is known as double descent. That further suggests a decrease in its LC and thus allows for training accurate models yielding small error growth rates in the flow solver. In this study, we investigate if double descent indeed occurs in the NN's generalization errors and LCs in the context data-driven turbulence modeling.
The exact determination of LCs for NNs is very expensive, though. Hence, one typically relies on upper and lower bounds. The tightness of these bounds decreases with increasing size of the NNs, which impedes our analyses. We therefore conduct a precursor study assessing the tightness of different popular bounds with varying NN sizes.

**Geometric Optimization in Machine Learning**
Müller, Johannes 09:10
*Technische Universtität Berlin, Germany*

We discusses an "optimize-then-project" approach for applications in scientific machine learning. The key idea is to design algorithms at the infinite-dimensional level and subsequently discretize them in the tangent space of the neural network ansatz. We illustrate this approach in the context of the variational Monte Carlo method for quantum many-body problems, where neural quantum states have recently emerged as powerful representations of high-dimensional wavefunctions. In this setting, we recover the celebrated stochastic reconfiguration algorithm, interpreting it as a projected Riemannian L2 gradient descent method. We further explore extensions to Riemannian Newton methods, and conclude with considerations related to the scalability of these schemes.

**First-order Optimization Methods for Functional Low-Rank Tensor Learning**
Klug, Nikolas 09:30
*University of Augsburg, Germany*

We consider first-order optimization methods for machine learning tasks with a functional low-rank tensor model, either based on rank-adaptive alternating optimization or parameterization-independent gradients. In particular, for polynomial classifiers we investigate the influence of bases on the learning dynamics and show how to obtain basis-independent descent directions. As illustrated by numerical experiments, this can considerably improve convergence.

**Riemannian Optimization on Tree Tensor Networks with Application in Machine Learning**
Willner, Marius (1,2); Trenti, Marco (2); Lebiedz, Dirk (3) 09:50
*1: University of Augsburg, Germany*
*2: Tensor AI Solutions, Germany*
*3: University of Ulm, Germany*

Tensor networks, originally developed for low-rank approximation and quantum simulations, have recently peaked interest as promising tools for kernel learning tasks. In this talk, we present a formal differential-geometric framework for tree tensor networks (TTNs) based on its quotient manifold structure, and show how it leads to efficient first- and second-order optimization algorithms. We also

introduce a backpropagation algorithm for kernel learning with TTNs and share some experimental results from a representative machine learning task.

**Certified Behavioral Coverage for Regression Neural Networks using Formal Methods**
Akhiat, Yassine; Grimm, Adrian; Cunis, Torbjørn; Daw, Zamira 10:10
*University of Stuttgart, Germany*

Deep neural networks are becoming widely used in complex systems, creating a need for simple and reliable methods to verify and certify their behavior especially in safety critical systems. CoVerNet is a new coverage-based testing approach that uses formally verified equivalence classes to give strong behavioral guarantees for neural networks. It was proposed to overcome the limitations of existing neural coverage methods, which often do not work well for testing and verifying neural network' behavior. CoVerNet showed promising results and was able to reveal how sufficient and adequate a given test suite is.

However, CoVerNet currently supports only classification problems. Many safety-critical applications use regression models, where the outputs are continuous instead of categorical. This makes CoVerNet's behavioral coverage metrics more difficult to apply. In this work, we extend CoVerNet to support regression neural network by redefining behavioral equivalence in terms of bounded output and introducing a new notion of *regression-aware behavioral coverage*. Instead of requiring identical outputs within an equivalence class, the extended framework verifies that all inputs inside a formally defined perturbation region lead to predictions within a safe region characterized by an upper bound to the neural network's local Lipschitz constant. The approach clusters the input space, generates regression-specific formal properties, and iteratively verifies each region using LipSDP to detect areas violating the required properties. We evaluate the extended CoVerNet on multiple regression tasks and demonstrate that it effectively uncovers robustness violations and the guide the testing toward the regions where more testing is needed. This work broadens the applicability of CoVerNet beyond classification, enabling its use in safety-critical regression applications.

## S25.01.2: Data-driven Microstructure Analysis and Homogenization

Date: March 17, 2026 08:30–10:30
Room: KII, M17.52
Chair(s): Schulz, Katrin

**An Integrated MD-NN-FE Optimization Framework for Carbon Nanotube Based Metamaterials**
Čanađija, Marko; Ivić, Stefan 08:30
*Faculty of Engineering, University of Rijeka, Croatia*

The dataset for training a partially input-convex neural network (PICNN) is obtained from an extensive set of molecular dynamics (MD) simulations. The MD simulations model uniaxial tension and compression tests of 818 single-walled carbon nanotubes (SWCNTs) of different chiralities and diameters at 300 K. The length-to-diameter ratio is approximately 5. The resulting stress-strain curves are used to train the PICNN, which then serves as a surrogate constitutive model for SWCNTs. However, because the MD tests are performed at 300 K, thermal vibrations are inevitably present and introduce self-excited oscillations in the SWCNTs, causing noise in the stress-strain curves. This noise can lead to violations of convexity of strain with respect to strain energy. In the PICNN, the strain energy must therefore be the output, while the inputs are the strain and the two parameters defining the chirality of the SWCNT. Training is performed on the differentiated version of the PICNN using stress–strain data points, ensuring that the model is automatically thermodynamically consistent. In addition to convexity, several other fundamental physical constraints are embedded in the neural network. The resulting network is implemented in the Abaqus UMAT subroutine, where it serves as the constitutive model for truss finite elements, with each truss element representing an SWCNT. In this way, all geometric and material nonlinearity procedures available in Abaqus can be used to model SWCNT-based nanotrusses. As a special case, an SWCNT nanostructure that represents a building block of

a metamaterial can be analyzed. Such a nanotruss-based metamaterial is expected to retain the favorable mechanical efficiency well-known from macroscopic truss structures. A verification example compares results obtained from MD and Abaqus for a simple spatial SWCNT nanotruss. The results clearly demonstrate that the new Abaqus implementation is as accurate as MD while being computationally much more efficient. This efficiency is essential for the final step, in which PICNN-driven simulations are coupled with the optimization framework to enable the optimal design of metamaterials with tailored properties. As examples, the maximization of stored elastic energy in an SWCNT nanotruss is performed, and an auxetic nanotruss structure is advanced to minimize the Poisson's ratio.

**Optimised Random Forest classifier for fibre tracking in a fibre orientation process**

Vaupel, Tim; Neethu, Ann Mary; Decke, Jens; Wünsch, Olaf 08:50
*Universität Kassel, Germany*

This work presents a fibre tracking process based on a Random Forest classifier, designed to work with very little labelled data while achieving robust performance. Unlike data-intensive AI methods, our approach focuses on careful feature selection and iterative optimization that improve the algorithm.

Fibre detection is formulated as a supervised classification task with two classes: fibre and background. Training begins with a small selection of annotated fibres and representative background areas. A significant improvement over previous work [1] is the deliberate selection of fibres that exhibit difficult variations in appearance – short fibres, poorly or differently exposed fibres, strongly curved fibres and overlapping fibres – so that even a compact set can adequately represent the variations required for reliable recognition. The background is modeled as a separate class. Strategic sampling enhances the separation between fibre and non-fibre areas. This has improved stability across images with different lighting and texture.

In this work we optimized the process, by evaluating different combinations of features across multiple patch sizes. An average ground truth mask was generated from optimal combinations of features and it was used for retraining the model. This significantly improved the detection of difficult fibre types and reduced false positive fibres in the background compared to our previous implementation. Beyond direct tracking, the approach can become a practical tool for data-intensive AI algorithms that require large annotated datasets.

Since this approach results in two classes (fibres and background), we have developed methods to separate the individual fibres from each other. We have implemented a graph based separation approach using skeletonisation of Random Forest generated mask and path scoring based on geometrical properties like length, curvature etc. This enables tracking of fibres in our experiment over a longer period of time using a small amount of annotated data, which contributes to determining the orientation of fibres in our experiment.

[1] Vaupel, T., Gerland, F., Schomberg, T., Wünsch, O. Advanced optical measurement techniques for simultaneous fibre orientation and flow analysis complemented by machine learning. Sci Rep 15, 38998 (2025). https://doi.org/10.1038/s41598-025-25656-3

**Combining Simulations and Experiments by a Data Fusion Approach: Image-Guided Analysis of Dislocation based Plasticity**

Bender, Julian (1,2); Schulz, Katrin (1,2) 09:10
*1: Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany*
*2: Karlsruhe University of Applied Sciences (HKA), Karlsruhe, Germany*

Dislocation based plasticity governs the evolution of microstructure and mechanical response in crystalline materials. A core challenge is to establish predictive models that derive characteristics of the microstructure directly from experimental observables. However, experimental characterization is time-consuming, expensive and the insights are limited by instrumental constraints e.g. to surface images and stress–strain data. In contrast, discrete dislocation dynamics (DDD) simulations offer insights into 3d dislocation microstructures with controllable, reproducible datasets. Moreover, the simulations provide direct access to physically relevant state variables that are typically inaccessible

in experiments. This motivates a data fusion approach that integrates complementary information from experiments and simulations to mitigate the limitations of each and to enable more robust, physically informed inference.

We present a workflow that links experimental data with synthetic data generated by DDD simulations. The approach follows a data fusion concept that combines raw or preprocessed experimental data with simulation data within a unified analysis pipeline. The proposed workflow is designed to be modular and extensible, allowing for the systematic integration of additional data modalities. We consider micro-compression tests with surface images and mechanical stress-strain data, while simulations deliver corresponding outputs enriched by dislocation densities and spatially resolved dislocation configurations across individual slip systems. Computer vision methods complement this integrated strategy. Synthetic DDD images were intentionally degraded to match the contrast and noise characteristics of surface measurements. A convolutional neural network (CNN) trained on this augmented dataset was then used to extract dislocation segments from noisy image data. Using the pre-trained model, we subsequently apply it to experimental data, enabling automated denoising and quantitative estimation of dislocation microstructures. This yields the basis for the incorporation of descriptors derived from stress–strain curves, ultimately enhancing data-driven predictions of plastic deformation mechanisms.

**Material Fingerprinting: A rapid optimization-free approach to material model discovery**

Martonová, Denisa (1,2); Kuhl, Ellen (1,2); Flaschel, Moritz (1,2) 09:30

*1: Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany*

*2: Department of Mechanical Engineering, Stanford University, California, United States*

Material Fingerprinting (MF) provides a fast, robust, and interpretable approach to identifying mechanical material models directly from experimental data, without solving optimization problems [1]. The method is based on the principle that each material exhibits a unique response under a standardized test. This response serves as the material's fingerprint, a compact signature reflecting its mechanical behavior. In an offline phase, a database is constructed linking fingerprints to specific well-known constitutive models. During the online phase, an unknown material is identified by measuring its stress-strain response, which is stored as a unique fingerprint. We then apply a pattern-recognition step based on cosine similarity to select the closest entry in the database. This approach eliminates the need for potentially non-convex optimization, providing high-speed, numerically stable, and transparent model selection.

We apply MF to experimental data in both supervised and unsupervised cases. Using data from rubber, hydrogel, and brain tissue, we demonstrate that MF correctly identifies suitable isotropic hyperelastic models for each material. In the supervised case, the identification process completes in less than one second on a standard personal computer. The selected models reproduce the full mechanical response with high accuracy, demonstrating that MF maintains both speed and fidelity across diverse material classes [2].

These results show that MF enables rapid and reliable model discovery, avoids numerical instability, and scales naturally to multi-modal datasets. Future work will focus on extending the approach to fully unsupervised workflows and more complex material behaviors.

[1] Flaschel M., Martonová D., Veil C., Kuhl E.: Material Fingerprinting: A shortcut to material model discovery without solving optimization problems. Computer Methods in Applied Mechanics and Engineering(2025). https://doi.org/10.1016/j.cma.2025.118573.

[2] Martonová D., Kuhl E., Flaschel M.: Material Fingerprinting for rapid discovery of hyperelastic models: First experimental validation. Journal of Mechanics and Physics of Solids (2025). https://doi.org/10.1016/j.jmps.2025.106463.

**Learning Microstructure-Property Relations in Foamed Concretes**

Eimke, Laurenz (1); Sadeghi, Seyed Reza (1,2); Caggiano, Antonio (2,3); Aldakheel, Fadi (1)

*1: Institute of Mechanics and Computational Mechanics (IBNM), Leibniz University Hannover, Appelstr. 9A, 30167 Hannover, Germany*
*2: Department of Civil, Chemical and Environmental Engineering (DICCA), University of Genoa, Via Montallegro, 1, 16145 Genoa, GE, Italy*
*3: LMNI, FIUBA, University of Buenos Aires, Argentina*

09:50

Foamed concretes are attractive thermal insulation materials due to their highly porous microstructure; however, their effective thermal conductivity is governed by complex interactions across multiple length scales that are difficult to capture using conventional homogenization approaches. Building on a previously developed representative volume element (RVE) generation framework for foamed concretes, realistic porous microstructures are generated and their effective thermal conductivity is numerically evaluated. Using this framework, a comprehensive database of porous RVEs and corresponding thermal conductivities is constructed, providing a rich foundation for data-driven analysis. Machine learning techniques, including a variational autoencoder (VAE) and a tandem neural network, are employed to elucidate the relationship between microstructural features and thermal conductivity. The predictive performance of models exploiting the full microstructural information is systematically compared with approaches relying on conventional descriptors such as porosity and pore size distribution. This comparison provides quantitative insight into the extent to which detailed microstructural characteristics can govern the effective thermal conductivity of foamed concretes.

## S25.02: Methods for Scientific Machine Learning

Date: March 17, 2026 16:30–18:30
Room: KII, M17.01
Chair(s): Stoll, Martin

**Data-intrinsic approximation in metric spaces**

Dölz, Jürgen (1); Multerer, Michael (2)

*1: University of Bonn, Germany*
*2: USI Lugano, Switzerland*

16:30

Analysis and processing of data is a vital part of our modern society and requires vast amounts of computational resources. To reduce the computational burden, compressing and approximating data has become a central topic. We consider the approximation of labeled data samples, mathematically described as site-to-value maps between finite metric spaces. Within this setting, we identify the discrete modulus of continuity as an effective data-intrinsic
quantity to measure regularity of site-to-value maps without imposing further structural assumptions. We investigate the consistency of the discrete modulus of continuity in the infinite data limit and propose an algorithm for its efficient computation. Building on these results, we present a sample based approximation theory for labeled data. For data subject to statistical uncertainty we consider multilevel approximation spaces and a variant of the multilevel Monte Carlo method to compute statistical quantities of interest. Our considerations connect approximation theory for labeled data in metric spaces to the covering problem for (random) balls on the one hand and the efficient evaluation of the discrete modulus of continuity to combinatorial optimization on the other hand. We provide extensive numerical studies to illustrate the feasibility of the approach and to validate our theoretical results.

**Reducing parametric problems with discontinuities using deep learning**

Chheda, Viral Paresh; Chasapi, Margarita

*RWTH Aachen University*

16:50

Model order reduction becomes necessary when dealing with large-scale engineering problems governed by parametric partial differential equations (PDEs). Conventional projection based reduced basis methods, e.g. based on proper orthogonal decomposition, are not only intrusive in nature but

may also demand tailored strategies to efficiently deal with non-linearities induced by the problem parameters [1]. Reducing the order of non-affine parametric problems while ensuring an efficient offline-online decomposition becomes more complicated if the solutions exhibit discontinuities. The nature of the problem itself, the type of parameters i.e. geometrical or physical, and the extent of their variations affect the complexity and reducibility of the problem. In this contribution we investigate non-intrusive and data-driven methods [2,3] to construct reduced order models that can be queried numerous times within few seconds while addressing the aforementioned issues. We are interested in scenarios with geometric and physical parameters, while targeting problems in fracture mechanics and inhomogeneous elasticity. Spline based discretizations to some parametric problems exhibiting the above-mentioned properties are used to benchmark the efficiency and accuracy of the reduced order models to be presented.

[1] Margarita Chasapi, Pablo Antolin, and Annalisa Buffa. "A localized reduced basis approach for unfitted domain methods on parameterized geometries." *Computer Methods in Applied Mechanics and Engineering* 410 (2023): 115997.

[2] Jan S. Hesthaven, and Stefano Ubbiali. "Non-intrusive reduced order modeling of nonlinear problems using neural networks." *Journal of Computational Physics* 363 (2018): 55-78.

[3] Nicola Franco, Andrea Manzoni, and Paolo Zunino. "A deep learning approach to reduced order modelling of parameter dependent partial differential equations." *Mathematics of Computation* 92.340 (2023): 483-524.

**Neural enrichment finite element method: A hybrid method for problems with strong oscillations or discontinuities**

Guo, Shihan; Richter, Thomas 17:10
*Otto Von Guericke Universität Magdeburg, Germany*

In this work, we propose a hybrid method, the Neural Enrichment Finite Element Method (NEFEM), deigned for problems involving strong oscillations or discontinuities. This method is based on gerneralized/extended FEM (GFEM/XFEM) framework, wherein neural networks (NNs) are introduced as enrichment functions for adaptivity, and the Ritz functional is applied for training process. The advancements are twofolds. First, the method constructs local subspaces with superior approximation properties, significantly reducing the required number of degrees of freedom (DoFs). Second, minimal a priori knowledge is required to define enrichment functions, as the NNs evolve heuristically during training. Moreover, we provide a residual-based error estimator and prove its reliability and efficiency. We also observe that the condition number of the system remains of the same order as that of standard FEM. The performance and effectiveness of the proposed method are validated through several numerical experiments.

**Data-driven reduced-order modeling for controlling dynamically-operated Power-to-X reactors**

Peterson, Luisa; Geschke, Alexander; Gosea, Ion Victor; Goyal, Pawan; Benner, Peter; Sundmacher, Kai 17:30
*Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*

Operator Inference (OpInf) is a scientific machine learning methodology that enables the construction of reduced-order models by learning the governing dynamics directly from data, thus bypassing the need for intrusive access to high-fidelity solvers. The workflow of OpInf encompasses two distinct stages: first, the high-dimensional state space is compressed onto a low-dimensional manifold; second, the dynamical operators governing this reduced space are inferred via regression. One challenge for OpInf is the robustness to experimental data (often corrupted by measurement noise), which, amongst others, severely degrades the finite-difference derivative estimates required for the standard implementation. To address this, we leverage a neural network surrogate within the OpInf framework, conceptually inspired by the DeepMoD (Deep learning based Model Discovery) algorithm. Instead of smoothing data and learning operators in separate steps, this hybrid approach performs both tasks jointly. A neural network approximates the continuous trajectory of the latent states, while

the quadratic operator structure of the reduced model serves as a physics-informed regularization. The training objective minimizes a composite loss function that balances the reconstruction of the projected measurement data with the physical consistency of the learned operators. This can be interpreted as an extension of the physics-informed neural networks (PINNs) philosophy, additionally leveraging the OpInf benefits. The learned OpInf-PINN model serves as the predictive core for the controlling step. By embedding the reduced-order dynamics as constraints in a nonlinear optimization problem, we maximize a performance metric while respecting operational boundaries. The case study focuses on a catalytic CO2 methanation reactor, pertaining to Power-to-X technologies for converting renewable electricity into synthetic fuels or platform chemicals. Power-to-X systems are essential for long-term energy storage and mitigating the mismatch between intermittent renewable generation and demand. We illustrate the robustness of the new method with respect to simulation data (corrupted with different levels of additive Gaussian noise), but also to purely experimental data.

**Physics based machine learning framework for cyclic damage evolution and fatigue lifetime-scale homogenization**

Baktheer, Abedulgader; Elasyed, Elsayed Saber; Aldakheel, Fadi 17:50
*Leibniz Universität Hannover, Germany*

Predicting structural lifetime under cyclic and fatigue loading is a major challenge in computational mechanics, especially for high-cycle fatigue problems in large-scale engineering systems such as aircraft, bridges, and wind turbines. Fatigue damage accumulation, crack initiation, and crack growth critically affect durability, yet direct mechanistic simulations over millions of cycles remain computationally prohibitive.

This work introduces a dual-model physics-based machine learning ($\varphi$ML) framework to capture both cycle-level fracture behavior and lifetime-scale fatigue evolution. One model predicts damage evolution throughout the full cyclic loading history, while the other operates at the lifetime scale, estimating accumulated damage over chunks of cycles. Both models employ double feed-forward neural networks guided by physical constraints, including energy balance, damage evolution, and degradation laws, ensuring physically consistent, interpretable, and generalizable predictions across unseen materials and loading scenarios.

Validation studies demonstrate that the models accurately reproduce nonlinear damage evolution under diverse loading histories and material parameters. The lifetime-scale model enables efficient high-cycle fatigue simulations by serving as a surrogate that jumps over multiple cycles without sacrificing accuracy, even in cases of complex, non-linear damage accumulation. This approach provides computationally efficient, scalable, and interpretable simulations of cyclic damage, enabling safer and more durable designs.

**REFERENCES**

[1] Aldakheel, F., Elsayed, E.S., Heider, Y. et al., Physics-based machine learning for computational fracture mechanics, Mach. Learn. Comput. Sci. Eng, 1, 18, 2025. https://doi.org/10.1007/s44379-025-00019-x.

[2] Baktheer A., Aldakheel F., Physics-based machine learning for fatigue lifetime prediction under non-uniform loading scenarios, Computer Methods in Applied Mechanics and Engineering, Vol. 444, 118116, 2025.

[3] Baktheer A., Mart´ınez-Pa~neda E., Aldakheel F., Phase-field cohesive zone modeling for fatigue crack propagation in quasi-brittle materials, Computer Methods in Applied Mechanics and Engineering, Vol. 422, 116834, 2024

**S25.02.2: Neural Networks with Mechanical Guarantees**

Date: March 17, 2026 16:30–18:30
Room: KII, M17.52
Chair(s): Cyron, Christian

**Neural Networks for Non-Convex Anisotropic Inelasticity at Finite Strains**

Holthusen, Hagen (1); Kuhl, Ellen (1,2)
*1: FAU Erlangen-Nuremberg, Germany*
*2: Stanford University, United States*

16:30

We introduce a thermodynamically consistent neural constitutive framework for finite strain anisotropic inelasticity that extends classical dual-potential formulations beyond convex potentials [1]. The method constructs the Helmholtz free energy and the dual inelastic potential on invariant sets derived from elastic, inelastic, and structural tensors, ensuring frame indifference, material symmetry, and independence of the intermediate configuration. Convexity and monotonicity constraints are embedded directly into the architecture by combining Input Convex Neural Networks with newly developed Input Monotonic Neural Networks, enabling the representation of non-convex but admissible dissipation potentials. To avoid instability of exponential-map integration during training, we introduce a Liquid Neural Network that approximates the implicit evolution of inelastic variables while preserving the multiplicative decomposition and positive definiteness of inelastic stretcches. After training, the physically consistent exponential update is reinstated for inference. The framework is evaluated using synthetic data generated from anisotropic finite-strain viscoelastic models and embedded into a finite element solver. Numerical studies at the material point and structural levels demonstrate accurate reproduction of stress responses, evolution of internal variables, and reaction forces, with robust extrapolation to unseen loading paths.

[1] Holthusen, H., & Kuhl, E. (2025). *A complement to neural networks for anisotropic inelasticity at finite strains*. arXiv. https://arxiv.org/abs/2510.04187

**Incremental (Contact) Approaches in Energy-Based Physics-Informed Neural Networks Using an Augmented Lagrangian Method**

Völkl, Simon; Wolff, Daniel; Popp, Alexander
*University of the Bundeswehr Munich, Germany*

16:50

Physics-Informed Neural Networks (PINNs) have recently emerged as a promising paradigm for solving partial differential equations (PDEs) by embedding governing physical laws into the loss function of neural networks. While standard PINNs are usually formulated based on the strong form of the PDE, energy-based PINNs (EPINNs) offer an alternative by bridging concepts from the principle of minimum total potential energy (PMTPE) and deep learning and instead incorporate the system's potential energy into the loss function. However, Energy-Based PINNs in contact mechanics, especially in incremental formulations, are just in an early investigation phase.

This work extends the EPINN framework towards geometrically nonlinear 3D contact mechanics by introducing an Augmented Lagrangian Method (ALM) for robust treatment of contact constraints. The incremental strategy solves a series of easier-to-solve nonlinear subproblems along the nonlinear load path and thus gives valuable insight into results of intermediate steps. The incorporation of ALM aims to improve the enforcement of the KKT-type inequality constraints, particularly the no-penetration condition as compared to simple approaches based on the penalty method.

The presentation will first outline the theoretical formulation of the incremental EPINN, which evaluates the total potential energy at the element level, and its integration with the ALM for contact mechanics. The devised implementation leverages a modern Python-based machine learning framework, enabling flexible GPU-accelerated training. Two representative benchmark problems are investigated: (i) a torsion test, designed to assess the model's performance on highly nonlinear deformation and stress states that are computationally demanding even for the traditional finite element method (FEM), and (ii) a Hertzian-type contact problem involving a hemisphere being in contact with a rigid plane, which highlights the accuracy of the proposed contact formulation.

All results are systematically compared to high-fidelity reference solutions obtained with the open-source FEM code 4C, demonstrating that the incremental EPINN can obtain accurate results while maintaining a computing time comparable to those of established methods.

**Physics-Augmented Surrogate Modelling for Multiscale Simulation of Battery Cells under Mechanical Abuse**

Dhumal, Harshwardhan (1,2); Goekuezuem, Felix Selim (1); Ricken, Tim (2) 17:10
*1: Daimler Truck AG, Germany*
*2: Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Pfaffenwaldring 27, Stuttgart 70569, Germany*

The growing focus on the development of electric vehicles with battery cells as alternative energy sources has sparked the need for assessing the mechanical integrity of the lithium-ion battery cells under abuse scenarios to ensure safety in automotive applications. Various macroscopic load cases, such as crush or impact, can lead to highly complex and intricate microstructural phenomena within the cell, that might potentially cause internal short circuits and thermal runaway. Such interactions between the macro- and micro-level can be captured using multiscale modelling methods. The traditional nested $FE^2$ homogenization techniques perform with good accuracy in large-scale simulations like full vehicle or battery pack crash analyses but are complex and computationally very expensive.

To tackle this issue, we propose a surrogate-based multiscale framework that significantly reduces computational cost while preserving microstructural fidelity. Initially, a high-fidelity Representative Volume Element (RVE) model of the battery cell's internal structure, i.e. the anode, cathode and separator layers, is employed to generate an extensive databank. This databank captures both microstructural details and homogenized stress-strain responses under various loading conditions. Utilizing this dataset, a Physics-Augmented Neural Network (PANN) [1] is developed that can replicate the behavior of a traditional constitutive material model. In contrast to the classical black-box machine learning approaches, the proposed model integrates continuum mechanics along with the corresponding physical constraints and constitutive principles, ensuring thermodynamic consistency and physical interpretability. This concept, also referred to as Constitutive Artificial Neural Networks (CANNs) [2], enables the surrogate to reproduce standard material modelling frameworks while maintaining data-driven adaptability.

This work is distinguished by the development of a physics-informed machine learning framework based on high-fidelity microstructural simulations, that exhibits good computational efficiency and physical consistency. The presented approach tends to bridge the gap between data-driven modelling and classical constitutive theory, allowing accurate stress predictions without iterative $FE^2$ computations. The potential impact is substantial, as machine learning based simulations of battery systems under crash scenarios can accelerate virtual safety assessments, reduce development costs, and support the design of safer electric vehicles.

**References**:

[1] Betim Bahtiri, Behrouz Arash, Sven Scheffler, Maximilian Jux, Raimund Rolfes, A thermodynamically consistent physics-informed deep learning material model for short fiber/polymer nanocomposites, Computer Methods in Applied Mechanics and Engineering, Volume 427, 2024, 117038, ISSN 0045-7825, https://doi.org/10.1016/j.cma.2024.117038

[2] Rosenkranz, M., Kalina, K.A., Brummund, J. et al. Viscoelasticty with physics-augmented neural networks: model formulation and training methods without prescribed internal variables. Comput Mech 74, 1279–1301 (2024). https://doi.org/10.1007/s00466-024-02477-1

**On Necessary and Sufficient Criteria for Compressible and Incompressible Polyconvex Hyperelastic Neural Network Material Models**

Geuken, Gian-Luca; Kurzeja, Patrick; Mosler, Jörn 17:30
*TU Dortmund, Germany*

In this talk, different necessary and sufficient criteria for hyperelastic, isotropic polyconvex material models are investigated, with a particular focus on neural network implementations. Different representations and the efficiency of the resulting models are analyzed, enabling an assessment of their practical applicability and providing insights into the underlying theoretical concepts. Convex Signed Singular Value Neural Networks (CSSV-NNs) [1] are applied to compressible materials – resulting in

a universal approximation framework for frame-indifferent, isotropic polyconvex energies – and are subsequently tailored to the incompressible case. In contrast, existing neural network approaches [2,3] ensure frame-indifference, isotropy and polyconvexity only by sufficient criteria that are overly restrictive. This is illustrated by numerical examples of well-established classical material models, including Neo-Hooke, Mooney-Rivlin, Gent, and Arruda-Boyce, as well as by Treloar's experimental data. In addition, a reduced variant of the CSSV-NN is discussed, for which the the numerical examples indicate that its underlying polyconvexity criterion may also be sufficient and necessary while being computationally more efficient.

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**Training of viscoelastic physics-augmented neural networks via full-field data**

Riemer, Brain M. (1,2); Kalina, Karl A. (1); Kästner, Markus (1)

*1: Institute of Solid Mechanics, TU Dresden, 01062 Dresden, Germany*
*2: Institute of Materials Chemistry, IFW Dresden, 01062 Dresden, Germany*

17:50

Within this contribution, we propose an unsupervised learning technique [1] for calibrating a physics-augmented neural network (PANN) [2,3,4] for small-strain viscoelasticity. In our framework, only data that can be measured in real macroscopic experiments are used for training. These are global test forces and surface displacements of the specimen. To implement the approach, we consider a thin sample under the assumption of a plane stress state. Using the equilibrium gap method in conjunction with a modern optimizer and automatic differentiation, a constrained optimization problem is formulated. We apply the proposed framework for the calibration of a PANN for isotropic small strain viscoelasticity [3]. This neural network-based approach relies on the theory of generalized standard materials (GSMs), which introduces two scalar-valued potentials such that the constitutive model is thermodynamically consistent by construction. Further physical principles, such as objectivity and material symmetry, are also encoded in the network architecture through invariant-based formulations of the respective potentials. The evolution of the internal variables is captured using an implicit time integration scheme, whereby a local Newton iteration is executed at every time step. To drastically reduce the required computational cost, the forward sensitivity method is applied instead of differentiating through all Newton iteration steps when computing the gradient of the target loss.

[1] P. Thakolkaran, A. Joshi, Y. Zheng, M. Flaschel, L. De Lorenzis, S. Kumar [2022]: "NN-Euclid: Deep-learning hyperelasticity without stress data", Journal of the Mechanics and Physics of Solids 169

[2] L. Linden, D. K. Klein, K. A. Kalina, J. Brummund, O. Weeger, M. Kästner [2023]: "Neural networks meet hyperelasticity: A guide to enforcing physics", Journal of the Mechanics and Physics of Solids 179

[3] M. Rosenkranz, K. A. Kalina, J. Brummund, W. Sun, M. Kästner [2024]: "Viscoelasticity with physics-augmented neural networks: model formulation and training methods without prescribed internal variables", Computational mechanics 74

[4] K. A. Kalina, J. Brummund, M. K¨astner [2025]: "A physics-augmented neural network framework for finite strain incompressible viscoelasticity", Preprint, https://doi.org/10.48550/arXiv.2511.02959

**Automated Finite Element Modeling of Anisotropic Viscoelasticity with Constitutive Artificial Neural Networks (vCANNs)**

Abdolazizi, Kian P. (1); Linka, Kevin (1,2); Cyron, Christian J. (1,3)
*1: Hamburg University of Technology*
*2: RWTH Aachen University*
*3: Helmholtz-Zentrum Hereon*

18:10

This contribution presents a unified and fully automated workflow for learning, calibrating, and implementing constitutive models of complex viscoelastic materials within finite element (FE) simulations. We employ viscoelastic Constitutive Artificial Neural Networks (vCANNs), a data-driven framework capable of representing anisotropic, nonlinear, viscoelasticity. Particular emphasis is placed on end-to-end automation, including robust generation of FE-ready material subroutines, enabling direct deployment in structural simulations without manual constitutive model development or implementation.

A key feature is the seamless integration of auxiliary material features—such as temperature, microstructural descriptors, or additional multi-modal data—directly into neural constitutive laws, enabling predictive viscoelastic material modeling. The framework is demonstrated on representative materials, including soft polymers with thermo-viscoelastic responses and anisotropic arterial tissue.

Performance in FE simulations is assessed through benchmark examples such as Cook's membrane and a three-dimensional arterial segment model. The results illustrate the flexibility, physical consistency, and numerical robustness of vCANNs, highlighting their suitability for automated, data-driven constitutive modeling in computational mechanics. All codes and FE subroutines required to apply the framework within the widely used commercial FE solver Abaqus are made openly available, facilitating the adoption of advanced viscoelastic neural material models in research and engineering practice.

## S25.03: Data-driven Models with Improved Sampling Efficiency

Date: March 18, 2026 08:30–09:30
Room: KII, M17.01
Chair(s): Schneider, Matti

**Reconfigurable computing in neural network-enhanced finite element analysis in structural dynamics**

Polydoras, Vasileios; Tandale, Saurabh; Stoffel, Marcus
*RWTH, Germany*

08:30

This study aims to integrate neural network-enhanced constitutive equations on Field Programmable Gate Arrays (FPGAs) during Finite Element simulations. In particular, classical constitutive equations governing material behavior are expressed by Neural Networks (NNs), which are subsequently embedded within Finite Element (FE) numerical simulations. The trained network architectures are mapped directly onto reconfigurable FPGA hardware, enabling a hardware–software co-design tailored specifically to the NN architecture. FPGAs show excellent capabilities in accelerating NN inference due to their flexibility in building dataflow datapaths that exactly describe NN inference, avoiding unnecessary instructions and memory overhead inherent to general-purpose processors, such as CPUs/GPUs, resulting in both high computational throughput and reduced energy consumption. FPGA is tailored specifically for the forward pass of the trained network, exploiting both fine-grained parallelism at the level of arithmetic operations and coarse-grained parallelism across NN layers, allowing multiple network operations to be executed concurrently in a deeply pipelined manner. The framework is applied to the dynamic analysis of impulsively loaded plate structures exhibiting strain-rate-dependent plasticity. A neural-network-based material description is integrated into an in-house FE formulation based on plate elements, enabling the efficient evaluation of constitutive responses at each Gaussian integration point during the simulation. The FPGA architecture is customized specifically for the trained NN, with the network topology, numerical precision, and dataflow optimized to

maximize performance and energy efficiency while maintaining sufficient accuracy for nonlinear dynamic simulations. Overall, the proposed approach demonstrates the potential of FPGA-accelerated NN constitutive models for FE simulations. This approach highlights the benefits of combining machine learning, computational mechanics, and reconfigurable computing for computationally efficient simulation frameworks.

**On Learning Gaussian Sobolev Operators with Near-Optimal Sample Complexity**

Adcock, Ben (1); Griebel, Michael (2,3); Maier, Gregor (2,3) 08:50
*1: Simon Fraser University, Canada*
*2: University of Bonn, Germany*
*3: Fraunhofer SCAI, Germany*

Operator learning has gained increasing research attention in recent years. Approximate operators, learned from data, hold promise to serve as efficient surrogate models for problems in computational science and engineering, complementing traditional numerical methods. Previous research efforts in understanding the underlying mathematical theory mainly focused on holomorphic operators and revealed that these can be learned efficiently: The worst-case approximation error scales algebraically or even exponentially with the reciprocal of the number of training samples.

We show that this data efficiency deteriorates if we consider less regular operators. More specifically, learning operators which are merely Sobolev regular with respect to a Gaussian measure exhibits an inherent *curse of sample complexity*: No method (polynomials, neural networks, kernel methods, etc.) to approximate such operators on infinite-dimensional domains based on $m$ (possibly adaptively chosen) linear samples can achieve algebraic convergence rates in $m$. This includes the important class of Lipschitz operators, which arise, e.g., as data-to-solution mappings in parametric variational inequalities. To assess the consequences of these asymptotic theoretical limitations for practical applications, we present a data-driven spectral algorithm for the recovery of Gaussian Sobolev operators from finitely many noisy point samples, which has near-optimal sample complexity. It is based on weighted least-squares approximation, does not require knowledge of the underlying Gaussian measure, and achieves higher convergence rates the smoother the operators are. We complement our theoretical analysis with numerical experiments.

**Generative material design with variational auto-encoders and hyperelastic neural network constitutive models**

Krämer, Niklas; Klein, Dominik K.; Roth, Fabian J.; Kannapinn, Maximilian; Weeger, Oliver 09:10
*TU Darmstadt, Germany*

We combine variational auto-encoders (VAEs) with hyperelastic physics-augmented neural network (PANN) constitutive models for generative design of microstructured materials. For this, we consider mechanical microstructured materials whose geometry depends on a high-dimensional parameter space. The VAE takes the high-dimensional parameter vectors for a wide range of different microstructures as input and maps them to a structured, low-dimensional latent space. In addition to the deformation state, the PANN constitutive model takes the values of the latent space as input and maps this onto a hyperelastic strain energy potential, from which then the stress state is derived. Overall, this architecture allows to map the geometry of a microstructure and the deformation state to the corresponding material properties, even for materials described by high-dimensional parameter spaces and with highly non-linear material behavior. Ultimately, this enables gradient-optimisation in the low-dimensional latent space to generate new microstructures with desired mechanical material behaviors. We demonstrate the applicability of the framework at the example of microstructured materials with a soft matrix that has several stiff, ellipsoidal inclusions of varying shape and orientation.

**S25.04: Neural Networks: Applications and Methodology**
Date: March 18, 2026 14:00–16:00
Room: KII, M17.01

**Sparse Training of Neural Networks based on Multilevel Mirror Descent**

Lunk, Yannick; Scott, Sebastian; Bungert, Leon 14:00
*Julius-Maximilians-Universität Würzburg, Germany*

We develop a sparse training algorithm for neural networks based on linearized Bregman iterations also known as mirror descent. The method alternates between static phases, in which the support of the parameters is fixed and adaptive phases, during which the full parameter vector is refined. This alternating scheme leverages the intrinsic sparsity-promoting dynamics of the linearized Bregman iterations.
To analyze the algorithm from a mathematical point of view, we embed this alternating procedure in a multilevel optimization framework.Using standard assumptions, we establish convergence of the partially stochastic algorithm. Furthermore, numerical experiments on benchmark datasets demonstrate that the algorithm produces highly sparse and accurate models.

**Error bounds for numerical integration in the context of neural network based modelling**

Mest, Felix; Arnold, Martin 14:20
*Martin-Luther-University Halle-Wittenberg, Germany*

Mechanical modelling often results in variational problems and differential equations, which can be difficult to solve efficiently. Neural networks provide a promising alternative to classical approaches in overcoming this problem [1]. An interesting approach, namely to learn the function to be integrated for obtaining a solution, was taken in [2]. In a classical setting, higher order Gaussian quadrature is used successfully for this problem class. The natural question that arises is: How well can neural network functions be numerically integrated?

In the case of approximating a function by a neural network, where we look to numerically integrate the resulting network function, the total error in the integral is composed of the approximation error and the quadrature error resulting from the numerical integration scheme. Classical schemes include the Newton-Cotes and Gaussian quadrature formulae. They come with a linear error functional. The Peano Kernel Theorem is a classical result for representing this functional in a form suitable to derive error bounds for smooth integrands, in the sense that they are sufficiently differentiable and have reasonable bounds on their derivatives. We show that it can easily be extended to the case, where derivatives have finitely many discontinuities or are of very large magnitude at finitely many points and derive error bounds from there.

Following the idea of [2], we train a neural network to minimize the L2 distance to Euler's elastica, reconstructed from a learned tangent angle function. We noticed that not considering higher order derivatives in the loss function may lead to small approximation error, but failure of numerical integration schemes to reach their theoretical order, while including smoothing terms may interfere with achievable approximation errors.

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[2] E. Celledoni, E. Çokaj, A. Leone, S. Leyendecker, D. Murari, B. Owren, R. T. Sato Martín de Almagro, and M. Stavole. Neural networks for the approximation of Euler's elastica. Computer Methods in Applied
Mechanics and Engineering, 435:117584, 2025.

**Regression model for a sensor-integrating jaw coupling that compensates for hyper-viscoelastic material behavior.**

Menning, Johannes Dieter Martin (1); Ewert, Arthur (2); Prokopchuk, Artem (3); Schlecht, Berthold (2); Vorrath, E.-F. Markus (3); Wallmersperger, Thomas (1)

*1: Institute of Solid Mechanics, TU Dresden, Germany*
*2: Institute of Machine Elements and Machine Design, TU Dresden, Germany*
*3: Institute of Semiconductors and Microsystems, TU Dresden, Germany*

14:40

In recent years, there has been an increased need to digitize production processes. In order to obtain the necessary data on these processes, numerous sensors must be installed on or in the machines. This can be difficult, especially when done retroactively, as the existing installation space must be able to accommodate the sensors. To address this issue, sensor-integrated machine elements are currently being developed. In these machine elements, the sensors are integrated directly into the respective element and thus enabling a space-neutral installation [1].

In the current work a sensor-integrating jaw coupling is investigated. The aim of this coupling is to measure the transmitted torque via measuring the deformation of the gear rim teeth. For this purpose, dielectric elastomer sensors (DESs), which change their capacitance when deformed, are employed. The functionality of this principle was shown e.g. in Ref. [2]. The gear rim material has viscoelastic properties. Thus, hysteresis occurs when plotting the torque (the measurand) versus the capacitance (the measured quantity). It follows, that to predict the torque based on the measured capacitance a regression model is needed. This purpose is achieved by using GRUs (Gated Recurrent Units), a type of recurrent neural network. The current capacity and the change in capacity over time are used as input variables. The sequence length and the other hyperparameters of the model were determined using the Python library 'Optuna'. The capabilities of the model were tested using experimental and numerical data. At the end, the model was successfully employed for real-time measurements of the sensor-integrating jaw coupling.

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**Multi-Headed Transformer Architectures as Time-dependent Wasserstein Gradient Flows**

Massucco, Alex (1); Del Grande, Leonardo (2); Carioni, Marcello (2); Brune, Christoph (2); Schönlieb, Carola-Bibiane (1)

*1: University of Cambridge*
*2: University of Twente*

15:00

In recent years, transformer architectures have revolutionized the field of language processing, opening the door to previously unforeseen possibilities. However, from a theoretical point of view, the mathematical models proposed in the literature often lack direct contact with the actual architectures and depend on strong simplifying assumptions. In this paper, we reduce this gap by modeling the data flow in multi-headed transformer architectures as time-dependent gradient flows for a suitable interaction energy capturing the design of the attention mechanism. The explicit dependence on time allows us to consider different weights for each head and for each layer, without imposing constraints on the initialization method. Moreover, we prove that the $\omega$-limit of the gradient flows are stationary points of the interaction energy functional. Finally, we analyze the stability of the gradient flows considering perturbations of both the initial data and the weights. Specifically, on the one hand, we study the robustness of the proposed models with respect to noisy inputs, establishing a continuous dependence of the gradient flows on the initial data and uniqueness of the flows. On the other hand, we prove the $\Gamma$-convergence of the perturbed interaction energy to the unperturbed one, leading to the convergence of the corresponding gradient flows.

**Machine Learning Based Virtual Sensor for the Shaft Torque during Helicopter Flight: Definition, Optimization and Uncertainty Analysis**

Kajolli, Jonida (1); Späth, Henry (2); Varchev, Tihomir (1); Daw, Zamira (2); Staudacher, Stephan (1) 15:20
*1: Institute of Aircraft Propulsion Systems, University of Stuttgart, Stuttgart 70569, Germany*
*2: Institute of Aircraft Systems, University of Stuttgart, Stuttgart 70569, Germany*

The shaft power off-take is a crucial parameter for controlling engine performance of helicopter turboshaft engines. It is usually measured using a dedicated physical sensor, which presents a possible single point of failure. Virtual sensors provide redundancy without relying on additional hardware. A data-driven virtual sensor for the power off-take of the shaft is introduced, that uses available in-flight measurement.

A physical analysis is performed to determine the variables relevant to the power off-take prediction. It is concluded that the data available through the existing in-flight measurements provides sufficient information to approximate the shaft power off-take with a virtual sensor. A neural network is employed as the core of the virtual sensor, which infers a mapping from the parameters of the physical analysis to an estimated shaft power off-take.

A proof of concept is shown with synthetic data, generated using a performance model of a turboshaft engine. These synthetic datasets include flight segments typical for a helicopter flight including hover and dynamic flight phases. It is shown that a sufficiently large dataset and a complex neural network lead to a satisfactory approximation of the power off-take.

The selection of neural network hyperparameters and the properties of the training dataset have an influence on the prediction quality. Consequently, the uncertainties in choosing the model hyperparameters and in the properties of the training dataset, along with their effect on the shaft power prediction, are investigated. In particular, different network architectures, learning rates and batch sizes, as well as the influence of dataset properties such as size, homogeneity and variety are compared and discussed.

Engine performance declines over the service life due to component degradation. Assessment of the virtual shaft power sensor for a deteriorating engine shows that the virtual sensor loses accuracy if it is not recalibrated regularly. The requirement for such an update fits the basic concept of digital twins. Recommendations are made for the update frequency and strategy.

**Multi-Fidelity CNN-Based Error Correction for Fast Thermal Runaway Prediction in High Voltage Battery Packs**

Ignatius, Anish Hilary; Armiti-Juber, Alaa; Keller, Karsten; Ricken, Tim 15:40
*University of Stuttgart, Germany*

Thermal design optimization of battery modules requires repeated transient simulations over a wide range of design parameters, which becomes computationally expensive when high-fidelity models are used. This work proposes a parametric reduced-order modeling framework that enables efficient and accurate thermal predictions for battery module design.
The temperature field is reduced using Proper Orthogonal Decomposition (POD), while the temporal evolution of the reduced coefficients is learned using a neural network. The model is trained to remain valid over a prescribed parameter space, enabling rapid evaluation of different design configurations. To improve accuracy in regions with strong temperature gradients, which are often poorly captured by standard reduced-order models, a weighted training strategy is introduced. Based on the magnitude of local temperature gradients, weights are dynamically assigned to critical spatial regions at each time step. These weights are used to scale the corresponding contributions in the neural network loss function, guiding the network to prioritize learning high-gradient regions. This approach enables the reduced-order model to better capture localized thermal behavior while maintaining computational efficiency.
The resulting reduced-order model is integrated into an optimization framework to identify optimal design parameters that satisfy thermal constraints and improve battery module performance. The

proposed approach is demonstrated on a battery module case study and the accuracy and computational cost is compared to conventional reduced-order model.

## S25.04.2: Constitutive Neural Networks

Date: March 18, 2026 14:00–16:00
Room: KII, M17.52
Chair(s): Kästner, Markus

### Automating constitutive modeling with LLMs

Tacke, Marius (1); Busch, Matthias (2); Abdolazizi, Kian (2); Eichinger, Jonas (1); Linka, Kevin (2); Cyron, Christian (1,2); Aydin, Roland (1,2) 14:00

*1: Helmholtz-Zentrum hereon, Germany*
*2: Hamburg University of Technology, Germany*

State-of-the-art approaches in constitutive modeling, such as constitutive artificial neural networks (CANNs), achieve high accuracy, strong generalization, and guaranteed adherence to physical constraints [1]. However, when modeling new materials, these methods often require deep expertise: Choosing the right approach, configuring the model, and performing effective hyperparameter optimization can be tedious and time-consuming for experts, and a significant barrier for non-experts.

This talk addresses this challenge by exploring the integration of large language models (LLMs) with CANNs. We present results on real-world datasets that capture strain–stress relationships for multiple hyperelastic materials under diverse loading scenarios [2]. These results demonstrate that CANNs generated and optimized autonomously by LLMs can match human-designed models in accuracy, generalizability, and physical consistency. Our approach not only accelerates constitutive modeling but also makes it accessible to a wider range of users.

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[2] Tacke, M., Busch, M., Abdolazizi, K. P., Eichinger, J. F., Linka, K., Cyron, C. J., Aydin, R. C. (2025). Automating modeling in mechanics: LLMs as designers of physics-constrained neural networks for constitutive modeling of materials. Under review. doi: https://doi.org/10.48550/arXiv.2512.01735

### Strategies to scale deep material networks for multiscale simulations of fiber reinforced composites

Bhat Keelanje Srinivas, Pavan (1,2); Kabel, Matthias (1); Schneider, Matti (1,2) 14:20

*1: Frauhofer ITWM, Germany*
*2: Institute of Engineering Mathematics ,University of Duisburg-Essen, Germany*

Fiber reinforced composites are versatile materials for light weight construction of industrial components. The characterization of these fiber-reinforced plastic components, taking into account variations in fiber orientation and volume fraction, is computationally challenging.

Using reduced order methods to replace traditional FFT simulations for scale bridging serves as an established approach for realizing multiscale simulations [1]. Lack of generalization to different material models, difficulty in extrapolation outside the training data distribution are some of the drawbacks of such models.

In recent years Deep Material Networks (DMNs) [2] have shown promise in providing a generalized workflow to deal with a large number of different material models. Most importantly the key idea of learning a complex microstructure with these material networks using linear elastic homogenization as a training data isolates the computational bottle neck encountered at the microscale. Once these networks are identified using machine learning methods, the elastic material nodes are switched to their inelastic behaviour during inference. Thus during inference the same material model and balance equations are solved for ensuring thermodynamic consistency of the predictions.

The current work starts with the state of art implementation of DMNs [3], applies it to fiber reinforced composites and discusses the associated strategies in scaling the DMNs to industrial scale multiscale simulations.

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**A physics-enhanced deep learning surrogate framework for elastoplastic material models**

Arora, Rishabh (1); Scheunemann, Lisa (1); Rezaei, Shahed (2); Brepols, Tim (1)

*1: Institute of Applied Mechanics, RWTH Aachen University*
*2: ACCESS e.V.*

14:40

Nonlinear material models with internal variables are central to the simulation of inelastic behavior in solids, yet their repeated evaluation in large-scale finite element analyses often represents a major computational bottleneck. Conventional return-mapping algorithms for elastoplasticity, viscoplasticity, or damage models are accurate and robust, but they can be costly when used in parameter studies or uncertainty quantification. This work presents a physics-enhanced deep learning surrogate framework for elastoplastic constitutive modeling, implemented in the JAX framework. For a particular set of boundary conditions and material properties, the proposed surrogate replaces the classical consitutive update with a neural network model that maps strains and internal variables at the beginning of a time step to plastic strain and updated internal variables at the end. The surrogate is trained via optimization of a multi-objective loss function that simultaneously accounts for the accuracy of plastic strain predictions and, the evolution of internal variables, and the satisfaction of thermodynamics requirements. Training data are generated from a uniform distribution in the sample space and reference material models under diverse loading paths, including multiaxial and non-proportional loading histories, to ensure a robust coverage of the relevant state space. The proposed framework is evaluated on representative nonlinear constitutive models and integrated into prototype finite element simulations. Its performance is assessed in terms of accuracy, stability under different loadings, and computational cost relative to standard return-mapping schemes. Numerical experiments show that the physics-enhanced surrogate can closely reproduce the reference material behavior while achieving substantial speed-ups, demonstrating its potential to accelerate nonlinear finite element simulations and support large-scale parameter studies as well as uncertainty quantification.

**A precise, efficient and flexible neural network model for strain-crystallizing rubber**

Friedrichs, Konrad; Dammaß, Franz; Kalina, Karl A.; Kästner, Markus

*Dresden University of Technology, Germany*

15:00

The self-reinforcing mechanism of strain-induced crystallization significantly influences the mechanical behavior of certain elastomers. In search of a suitable model for this inelastic phenomenon, we propose a continuum-mechanical two-potential framework based on generalized standard materials (GSMs) [1]. Therein, we pursue a physics-augmented neural network (PANN) approach to flexibly describe the required energy and dissipation potentials. In doing so, we ensure that any discovered material law fulfils essential physical principles, including objectivity, isotropy and thermodynamic consistency. The evolution law for the crystallinity is derived from the two potentials as a classical GSM-type equation with two additional Lagrange multipliers and associated Karush-Kuhn-Tucker conditions. Thus, boundedness of the degree of crystallinity is ensured while maintaining thermodynamic

consistency, thereby allowing its interpretation as a concentration-type variable. We equivalently derive the governing model equations and the field equations in a time-discrete setting from an incremental variational framework, providing a basis for a finite element implementation. We evaluate the PANN on experimental stress and crystallinity data for unfilled rubber, where very good agreement is found for the training data, as well as satisfactory generalization behavior for unseen deformation sequences. Similarly, reasonable field distributions of both stress and crystallinity are computed for a notched specimen, demonstrating the model's applicability for deformation states of arbitrary complexity. Further, the flexibility of the PANN is demonstrated by employing it for carbon black-filled natural rubber, achieving similar performance.

[1] K. Friedrichs, F. Dammaß, K.A. Kalina, M. Kästner. Precise, efficient and flexible modeling of crystallizing elastomers based on physics-augmented neural networks. arXiv-Preprint, 2025. arXiv:2511.14553

**Inelastic Constitutive Kolmogorov-Arnold Networks: A Generalized Framework for Automated Discovery of Interpretable Inelastic Material Models**

Ji, Chenyi (1); Abdolazizi, Kian P. (2); Holthusen, Hagen (3); Cyron, Christian J. (2,4); Linka, Kevin (1) 15:20

*1: Computational Mechanics for Medicine, Institutes of Applied Medical Engineering, RWTH Aachen University, Germany*
*2: Institute for Continuum and Material Mechanics, Hamburg University of Technology, Germany*
*3: Institute of Applied Mechanics, University of Erlangen-Nuremberg, Germany*
*4: Institute of Material Systems Modeling, Helmholtz-Zentrum Hereon, Germany*

The rapid progress of automated and interpretable material model discovery using machine learning has significantly advanced data-driven constitutive modeling. In this context, Kolmogorov–Arnold Networks (KANs) provide substantially enhanced transparency compared to conventional multilayer perceptrons and have demonstrated strong potential in computational mechanics, including the discovery of hyperelastic material models.

In this talk, we introduce inelastic Constitutive Kolmogorov–Arnold Networks (iCKANs), building upon a generalized constitutive framework for inelastic materials. Our formulation combines the flexibility of data-driven modeling with the intrinsic interpretability of KANs, enabling the identification of human-readable inelastic constitutive laws. To explicitly recover interpretable material representations, we employ symbolic regression techniques to express both the strain energy function and the dissipation potential in closed mathematical form.

We evaluate the proposed framework using synthetic data as well as experimental viscoelastic datasets for the polymeric materials VHB 4910 and VHB 4905. The results demonstrate that iCKANs accurately capture complex viscoelastic behavior while preserving physical interpretability. Moreover, the framework naturally accommodates additional material features, such as temperature dependence, highlighting its potential as a transparent and extensible approach for data-driven inelastic material modeling.

**Data-Driven Surrogate Modelling of Hydrogen Tank Crash Response using Neural Networks**

Ramachandran, Achyuth; Keller, Karsten; Ricken, Tim 15:40

*Institut für Statik und Dynamik der Luft- und Raumfahrtkonstruktionen, Universität Stuttgart, Germany*

Hydrogen storage systems in electric vehicles require rigorous crash assessment, performed using high-fidelity finite element simulations. While these simulations provide detailed mechanical insight, their high computational cost limits their applicability in rapid optimization/validation studies and iterative design processes. Computationally efficient surrogate models are therefore of growing interest in engineering.
In this work, we present a hybrid data-driven, physics-aware neural network for predicting spatio-temporal displacement and stress fields of a hydrogen storage tank subjected to side pole impact crash scenarios. Multiple model architectures with spatial and temporal learning capabilities are considered, including graph-based models, convolutional neural networks and conventional multilayer

perceptrons. The model is trained on a dataset of 150 crash simulations (simulation time of 50 milliseconds split into 27 timesteps) spanning impact velocities from 28 – 41 km/h, impactor masses from 1400 – 2400 kg, impact angles of 75° and 90°, and four distinct impact positions along the chassis. Physics-based constraints are incorporated into the learning process to promote mechanically consistent predictions on the displacement components and Cauchy stress tensor using the resultant displacement and the von Mises stress respectively.
A comparative evaluation is conducted between the proposed surrogate models and conventional finite element simulations, with emphasis on computational efficiency, qualitative agreement in predicted fields, and robustness across loading scenarios. This study illustrates how physics-aware machine learning approaches can complement established numerical methods and support more efficient analysis and design of hydrogen storage systems.

## S25.05: Data-driven Methods for Dynamical Systems

Date: March 18, 2026 16:30–18:30
Room: KII, M17.01
Chair(s): Weeger, Oliver

### Parametric Symplectic Neural Networks

Janik, Konrad (1); Benner, Peter (1,2) 16:30
*1: Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg, Germany*
*2: Otto von Guericke University Magdeburg, Germany*

The numerical integration of Hamiltonian systems is a central topic in computational physics and theoretical chemistry. Intrinsic structure-preserving symplectic networks (SympNets) [1] are a widely used tool when it comes to learning symplectic integrators for Hamiltonian systems from data. More often then not, Hamiltonian systems of interest depend on a set of parameters. Currently, SympNets do not respect parameters. Therefore, SympNets have to be retrained for every new parameter combination. To eliminate this necessity, we propose to extend the SympNet architecture to handle parameters explicitly, making it suitable for parametric Hamiltonian systems. This approach is coined ”ParSympNets”. We perform different numerical experiments to investigate the approximation and generalization capabilities of ParSympNets. Furthermore, we present a new universal approximation theorem, which shows that ParSympNets can approximate arbitrary parametric symplectic maps.

[1] P. Jin, Z. Zhang, A.Zhu, Y.Tang, and G. E. Karniadakis. SympNets: intrinsic structure-preserving symplectic networks for identifying Hamiltonian systems. Neural Networks, 132:166–179, 2020. doi:10.1016/j.neunet.2020.08.017.

### Learning Stable port-Hamiltonian Dynamics with Neural Networks

Roth, Fabian J. (1); Kannapinn, Maximilian (1); Klein, Dominik K. (1); Peters, Jan (2); Weeger, Oliver (1) 16:50
*1: Cyber-Physical Simulation - TU Darmstadt, Germany*
*2: Intelligent Autonomous Systems - TU Darmstadt, Germany*

Accurate and computationally efficient surrogate and reduced-order models are a key enabler for the data-driven analysis, design, and optimization of complex engineering systems. While purely data-driven machine learning models are efficient, they often suffer from limited robustness, poor extrapolation, and a lack of physical interpretability, particularly in small-data regimes. Scientific machine learning addresses these limitations by integrating mathematical structure and physical principles directly into learning architectures.
This contribution presents stable port-Hamiltonian Neural Networks (sPHNNs) [1] as a physics-aware machine learning framework for nonlinear dynamic system identification and surrogate modeling. The approach combines the port-Hamiltonian formalism from dynamical systems theory with neural network approximation to learn low-dimensional nonlinear state-space models from data. Conservative and dissipative dynamics are represented explicitly through a learned Hamiltonian energy

function and structurally constrained interconnection and dissipation operators. By enforcing an energy balance relation and convexity constraints on the Hamiltonian, the model guarantees Lyapunov stability and bounded trajectories by construction and ensures global asymptotic stability in strictly dissipative settings. Furthermore, the architecture can incorporate interactions with the environment through external inputs.
From a computational and mathematical perspective, sPHNNs embed stability and thermodynamic consistency as hard constraints within a flexible learning architecture. These guarantees enable robust generalization from sparse or noisy data and prevent non-physical behavior commonly observed in unconstrained neural network models. Numerical experiments on real-world benchmark datasets demonstrate improved accuracy and stability compared to purely data-driven alternatives.
Evaluation with real-world benchmark data demonstrates the sPHNN's ability to generalize from sparse data, outperforming the purely data-driven approach and avoiding instability issues. In addition, the model's potential for data-driven reduced order modeling is highlighted by training it on multi-physics simulation data to construct a surrogate model. When utilizing augmented dimensions [2], the stability constraint enables a safe and stable exploration of the added flexibility. While sPHNNs are confined to modeling globally stable systems, in their applicable domain, they promote robustness and physically plausible dynamics.
[1] Roth, F. J., Klein, D. K., Kannapinn, M., Peters, J., and Weeger, O. Stable Port-Hamiltonian Neural Networks. Accepted at Advances in Neural Information Processing Systems, volume 38 (2025). Preprint at https://doi.org/10.48550/arXiv.2502.02480 (2025).
[2] Dupont, E., Doucet, A., and Teh, Y. W. Augmented neural odes. Advances in Neural Information Processing Systems, volume 32, (2019).

**Integration of Physics-Augmented Neural Networks for Explicit Dynamics in OpenRadioss**
Maurer, Lukas; Ilchi, Mehrshad; Eisenträger, Sascha; Juhre, Daniel 17:10
*Otto von Guericke University Magdeburg, Germany*

Data-driven modeling techniques have gained significant attention due to their ability to capture the complex constitutive behavior beyond the limitations of classical material models. Physics-augmented neural networks (PANNs), which embed physical constraints directly into their architecture, combine the flexibility of deep learning with the reliability required for engineering simulations. Hence, they have found widespread use in computational mechanics.

This work presents an approach to integrate such network architectures into the open-source explicit finite element solver OpenRadioss (Altair). Despite being commonly used for crash and impact simulations, we focus on the integration of advanced neural network-based hyperelastic constitutive laws. To this end, a framework to transfer pre-trained network architectures and their corresponding parameters is developed. These networks are trained using the PyTorch toolbox, but the proposed procedure can easily be adapted to other machine learning frameworks, e.g., TensorFlow. The key advantage of our approach is that it enables direct use of all algorithms and finite element technologies available in OpenRadioss, without requiring the development of specialized solvers.

Verification examples demonstrate the ability of PANNs to accurately reproduce the nonlinear large-strain behavior characteristic of hyperelastic materials. Overall, the presented framework paves the way for future applications of machine learning-based constitutive modeling in industrial simulation pipelines. Moreover, it highlights how open-source tools such as OpenRadioss can serve as a testbed for next-generation physics-based neural networks.

**Symplecticity-Preserving Prediction of Hamiltonian Dynamics by Generalized Kernel Interpolation**
Herkert, Robin; Ehring, Tobias; Haasdonk, Bernard 17:30
*University of Stuttgart, Germany*

We propose a kernel-based surrogate for integrating Hamiltonian dynamics that is symplectic by construction and tailored to large prediction horizons. The approach targets fast and reliable long-time

simulation when classical structure-preserving time stepping becomes expensive due to accuracy requirements leading to small-step size restrictions.

Our method learns a differentiable scalar potential whose gradient enters a symplectic-Euler update. The resulting discrete flow map is symplectic and therefore exactly preserves the canonical symplectic structure. Rather than approximating the physical Hamiltonian itself, training focuses on matching the gradient information required by the symplectic update over a prescribed macro time step.

Learning is formulated as a gradient Hermite–Birkhoff interpolation problem in a reproducing kernel Hilbert space. This yields a systematic framework which is used for deriving error control and convergence statements for the resulting symplectic predictor. Greedy sparsification strategies are employed to construct compact surrogate models while retaining rigorous approximation guarantees.

Algorithmically, the symplectic kernel predictor is combined with symplectic model order reduction, enabling efficient treatment of high-dimensional systems arising, for example, from spatially discretized Hamiltonian PDEs. This leads to an offline–online workflow: high-fidelity data are generated with a trusted symplectic integrator at fine step sizes offline and are compressed using symplectic model order reduction, while online evaluation uses a single implicit symplectic-Euler–type solve per macro step driven by the learned kernel potential.

Numerical tests for a pendulum, a nonlinear spring–mass chain, and a semi-discrete wave equation demonstrate the efficiency of the approach. For the same macro time step, long-time trajectory errors are reduced by two to three orders of magnitude compared to an implicit midpoint baseline with the same macro time step, while maintaining robust qualitative behavior even outside the training domain. The presentation will outline the theoretical guarantees and highlight when the method is most advantageous in long-horizon forecasting.

**Deciphering Acoustic Emission of Microsamples with Machine Learning**

Ispánovity, Péter Dusán (1); Berta, Dénes (1); Katzer, Balduin (2,3); Schulz, Katrin (2,3) 17:50

*1: ELTE Eötvös Loránd University, Hungary*
*2: Karlsruhe Institute of Technology, Institute for Applied Materials (IAM), Karlsruhe*
*3: Hochschule Karlsruhe - University of Applied Sciences (HKA), Karlsruhe, Germany*

Plastic deformation in crystalline materials is highly intermittent on the micron scale and proceeds through discrete slip events with a broad range of sizes. Two experimental techniques are commonly used to study this behaviour: microcompression testing of small-scale samples and acoustic emission (AE) measurements. While AE provides high-frequency time-resolved data, its quantitative interpretation remains challenging due to the complexity and volume of the recorded signals.

In the first part of this work, we combine microcompression and AE measurements in a single experimental setup to establish a direct link between mechanical response and acoustic activity. Zn single-crystal micropillars oriented for basal slip are compressed in situ inside an SEM while mounted on an AE sensor. We observe a clear one-to-one correspondence between stress drops in the force–displacement curves and individual AE events, providing a reliable experimental basis for interpreting AE signals in terms of underlying plastic activity.

In the second part, we focus on **data-driven analysis of AE signals using machine learning**. From the raw AE waveforms, we extract a set of statistical and spectral features that describe the signal amplitude, frequency content, and temporal structure. Supervised machine learning models are then trained to reconstruct key aspects of the mechanical response, including the force–time evolution and the occurrence and magnitude of slip events, using AE data alone. The models show good predictive performance and remain robust when applied to samples of different sizes.

The results demonstrate that AE signals contain sufficient information to quantitatively predict plastic deformation behaviour when analyzed with appropriate machine learning methods. This work

highlights the role of feature extraction, regression models, and validation strategies in linking high-frequency experimental data to mechanical observables, and illustrates how machine learning can support the interpretation of complex datasets in experimental mechanics.

## S25.06: Operator Learning and Graph-based Methods

Date: March 19, 2026 08:30–10:30
Room: KII, M17.01
Chair(s): Fritzen, Felix

### Graph-based automatic detection of deformations in FEM simulations

Bizzotto, Emanuele; Fender, Johannes; Krischer, Lukas; Kutyniok, Gitta 08:30
*BMW, Germany*

The post-processing of FEM simulations is often a time-consuming and repetitive task, involving lengthy manual operations to detect and quantify deformed regions with respect to criticality, while also dealing with noise. In this talk, we present a novel method for the automatic detection and classification of deformations in a mechanical body using machine learning within the context of dynamic FEM simulations. Most state-of-the-art methods for deformation and damage assessment of real objects rely on the analysis of 2D images. In contrast, the proposed approach operates directly on the 3D FEM mesh. The 3D information is converted into a graph, initially preserving only nodal curvature change and thereby making the process mesh-independent. Graph Signal Processing (GSP) and standard deep learning are employed to extract meaningful information from the data. Furthermore, rather than using a black-box deep learning model — where tasks are solved by a large, unexplainable neural network — our approach decomposes the problem into a sequence of simpler, well-understood steps, each addressed by tailored algorithms. Description, detection and classification of different deformation classes are demonstrated and validated on synthetic datasets.

### Generalizable Graph Neural Networks for Hemming Simulations achieved by inducing Rotational-Invariance and Scale-Normalized Features and Multi-Scale Training

Paramasivam, Naveen (1,2); Shibil, Muhammed (3); Yazdani, Saleh (1); Wagner, Marcus (2) 08:50
*1: BMW Group, Munich, Germany*
*2: OTH Regensburg, Regensburg, Germany*
*3: TH Ingolstadt, Ingolstadt, Germany*

Recently,Graph Neural Networks (GNN) are being used as surrogate models for the Finite Element (FE) simulations in various applications. In sheet metal forming, stress-tensors through the thickness of a geometry can be predicted by GNN, thereby serving as effective surrogate models for FE simulations. However, GNNs suffer from coordinate- and dimension-dependency, limiting their efficiency in predicting the geometries, that are scaled or rotated in global coordinates. Although dimension- and rotation-invariant GNNs have been studied extensively, application-specific challenges demand tailored adaptations and improvements. In hemming simulations of automotive parts, where deformations primarily occur along the geometry's perimeters, rotation-invariance and scale equivariance need to be customized for this context. This study proposes a generalizable GNN model for rotation and scaling which can predict the stress-tensors of a hemmed sheet metal, subjected to different ranges of rotation or scaling about different axes in any coordinate system.

The fundamental graph structure for the GNN was constructed using nodal coordinates obtained from the results of hemming simulations performed using a FE solver. To incorporate rotational invariance, all coordinate-dependent inputs were replaced with rotation-invariant geometric attributes. Specifically, Euclidean distances, angular relationships, curvature, and additional edge-based features were computed to ensure that the GNN receives consistent information regardless of the geometric orientation of sheet metals. Scale-normalization was similarly achieved by normalizing all the global geometric parameters using a characteristic length derived from Principal Component Analysis (PCA), while local shape features were made non-dimensional based on a node-wise neighborhood scale. In addition, explicit scaling parameters were used to improve dimensional awareness of the GNN

and reduce the dependency on absolute part size or mesh resolution. The GNN was then trained on a diverse multi-scale dataset of FE-based hemming simulations to predict stress tensors at each integration point through the thickness of the sheet metal.

Overall, incorporating rotation-invariant geometric attributes, scale-normalized nodal features, explicit scaling parameters and a multi-scale training dataset enabled the proposed GNN to learn scale- and rotation-dependent physical relationships more effectively than the baseline. Although the GNN architecture does not enforce strict rotation invariance or scale equivariance, these design choices introduce a strong inductive bias towards rotation or scale awareness, yielding improved generalization across geometries of varying rotations and sizes. This indicates that explicit scale conditioning, rotational invariance in the inputs, and multi-scale supervision offer a practical and efficient pathway to more robust deep learning surrogate models for FE simulation.

**Surrogate-based topology optimization using graph neural networks**

Gündoğan, Elif; Duddeck, Fabian
*Technical University of Munich, Germany*

09:10

Topology optimization is commonly used in lightweight design. Among the available approaches, the Moving Morphable Components (MMC) method [1] represents the topology based on the evaluation of level-set functions associated with each component. Compared to density-based formulations, MMC significantly reduces the number of design variables, enabling the use of population-based optimization algorithms for problems where gradient information is unavailable. However, population-based algorithms generally require more finite element (FE) evaluations, which motivates the use of a surrogate model to approximate the objective function with low computational effort.

Graph neural networks (GNNs) are novel deep learning architectures that operate on graph-structured data and have recently gained attention as effective surrogate models for complex simulations. Their inductive bias helps them learn local interactions between neighbors, improving generalization to unseen geometries. GNNs have been successfully applied to predict both graph-level quantities, such as homogenized material properties, as well as node-level outputs like stress and strain fields [2]. They can also capture abstract connections between entities. For example, UV-Net [3] uses the face adjacency graph of CAD geometries to create complex 3D shape representations.

This contribution offers a novel representation for the MMC parametrization using graphs, where geometry and boundary conditions of the components are encoded into node features. A GNN based on UV-Net is trained on MMC-based structures to predict compliance in a cantilever beam problem. The GNN utilizes the permutation-equivariant nature of MMC, aiming to reduce the high data requirements in the training phase. By avoiding the expensive FE evaluations and capturing spatial relationships through graph connectivity, a significant speedup during the optimization phase is achieved.

References

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[3] Jayaraman P. K., Sanghi A., Lambourne J. G., Willis K. D. D., Davies T., Shayani H., Morris N., UV-Net: Learning from boundary representations, arXiv preprint (2021). https://doi.org/10.48550/arXiv.2006.10211

**Physics-informed learning of the solution operator of three-dimensional microstructures**

Eivazi, Hamidreza (1); Tröger, Jendrik-Alexande (2); Hartmann, Stefan (2); Wessels, Henning (1) 09:30

*1: Institute of Applied Mechanics, Division Data-Driven Modeling of Mechanical Systems, Technische Universität Braunschweig, 38106 Braunschweig, Germany*

*2: Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany*

Learning solution operators for microstructural problems is of central importance in multiscale simulations, where microscale physics can be replaced by surrogate models to reduce computational cost. In this work, we extend the Equilibrium Neural Operator (EquiNO) [1] as a physics-informed PDE surrogate for predicting three-dimensional displacement and stress fields. The proposed framework is tailored to multiscale $FE^2$ computations and combines concepts from reduced-order modeling and physics-informed operator learning to achieve efficient and accurate surrogates. By construction, EquiNO satisfies the balance of linear momentum by projecting the solution onto a set of divergence-free basis functions obtained via proper orthogonal decomposition. Furthermore, the computational cost of training is significantly reduced by selecting a set of so-called magic points using the discrete empirical interpolation method [2], enabling the model to be trained only on a small number of spatial locations. The method is applied to quasi-static solid mechanics problems. Numerical results demonstrate that the proposed approach can be trained efficiently and delivers accurate predictions even when trained on small datasets.

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**Global Graph Surrogates and Neural Graph Elements for Computational Mechanics**

Gulakala, Rutwik; Stoffel, Marcus 09:50

*RWTH Aachen, Germany*

Machine learning surrogates are increasingly used to accelerate physics-based simulations by predicting full-field responses at a fraction of the computational cost [1,2]. Recent generative and graph-based approaches demonstrate that FE field variables can be inferred directly from mesh-based inputs and boundary conditions, enabling fast approximation of stresses and strains on discretized domains [1,3]. In parallel, graph-network-enhanced formulations provide a natural representation of FE connectivity and locality, motivating mechanics-aware learning architectures that align with the FE discretization principle [1,3,4]. In this contribution, we first present a global surrogate workflow for predicting displacement and stress fields of a three-dimensional automotive bumper problem. The models are trained on geometrically nonlinear, inelastic FE simulation data [5]. While accurate within the training distribution, global models remain tightly coupled to problem dynamics, geometries, and loading configurations. To address this, we introduce the concept of Neural Graph Elements (NGEs): localized graph-based neural operators that learn element-level mechanical behavior rather than structure-specific solution fields. This modular formulation supports the assembly of complex structures from reusable learned elements, offering a pathway toward transferable, mesh-robust surrogates and a closer integration of data-driven modeling with numerical methods in mechanics.

References

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[2] M. Stoffel, R. Gulakala, F. Bamer, and B. Markert, "Artificial neural networks in structural dynamics: A new modular radial basis function approach vs. convolutional and feedforward topologies," *Computer Methods in Applied Mechanics and Engineering,* no. 364, p. 112989, 2020.

[3] R. Gulakala, V. Bhaskaran, M. Stoffel, *A generative learning and graph-based framework for computing field variables in Finite Element simulations*, CMAME 428, 117111, 2024.

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**A spike-based graph surrogate for modeling finite element structures**

Bhaskaran, Vaishnav; Gulakala, Rutwik; Stoffel, Marcus 10:10
*RWTH Aachen University, Germany*

The use of Artificial Intelligence in structural mechanics has grown substantially in recent years, especially employing surrogate models to replace finite element simulations entirely. In this context, Graph Neural Networks (GNNs) have emerged as a particularly effective class of models, as their graph-based formulation naturally represents unstructured domains such as finite element meshes. Analogous to the assembly of global responses from local element contributions in the finite element method, GNNs operate through localized message passing between neighboring nodes, making them well suited for learning finite element operators.

In this work, we investigate graph-based surrogate models for fundamental finite element structures, focusing on the prediction of structural deformations exhibiting both elastic and plastic behavior. The proposed approach leverages local message passing to model physical and geometrical nonlinearities. While conventional GNNs demonstrate strong predictive performance, their training and inference stages are associated with considerable energy consumption. To address this limitation, we explore the integration of spiking neural networks into the graph learning paradigm, motivated by their event-driven computation and potential for energy-efficient execution.

We propose a spike-based graph neural model and evaluate its performance against a non-spiking counterpart in terms of predictive accuracy and computational characteristics. Furthermore, we compare the energy consumption profiles of both models by deploying them on neuromorphic framework, highlighting the potential of spiking graph-based models for sustainable surrogate modeling in computational mechanics.

## S25.07: Data-driven Methods for Inverse Problems and Uncertainty Quantification

Date: March 19, 2026 14:00–16:00
Room: KII, M17.01
Chair(s): Fritzen, Felix
Eidel, Bernhard

**Analyzing Uncertainty Quantification in Statistical and Deep Learning Models for Probabilistic Electricity Price Forecasting**

Lebedev, Andreas (2); Das, Abhinav (2); Pappert, Sven (3); Schlüter, Stephan (1) 14:00
*1: Ulm University of Applied Science, Ulm, Germany*
*2: Ulm University, Ulm, Germany*
*3: TU Dortmund, Dortmund, Germany*

Precise probabilistic forecasts are fundamental for energy risk management, and there is awide range of both statistical and machine learning models for this purpose. Inherent to these probabilistic models is some form of uncertainty quantification. However, most models do not capture the full extent of uncertainty, which arises not only from the data itself but also from model and distributional choices. In this study, we examine uncertainty quantification in state-of-the-art statistical and deep learning probabilistic forecasting models for electricity price forecasting in the German market. In particular, we consider distributional deep neural networks (DDNNs) and augment them with an ensemble approach, Monte Carlo (MC) dropout, and conformal prediction to account for model uncertainty. Additionally, we consider the LASSO-estimated autoregressive (LEAR) approach combined with quantile regression averaging (QRA),generalized autoregressive conditional heteroskedasticity (GARCH),

and conformal prediction. Across a range of performance metrics, we find that the LEAR-based models perform well in terms of probabilistic forecasting, irrespective of the uncertainty quantification method. Furthermore, we find that DDNNs benefit from incorporating both data and model uncertainty, improving both point and probabilistic forecasting. Uncertainty itself appears to be best captured by the models using conformal prediction. Overall, our extensive study shows that all models under consideration perform competitively. However, their relative performance depends on the choice of metrics for point and probabilistic forecasting.

**Application of deep symbolic regression for approximation problems in statistical mechanics.**

Popova, Alina (1,2); Abdusalamov, Rasul (1); Itskov, Mikail (1,3) 14:20

*1: Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany*
*2: School of Mathematical and Statistical Sciences, University of Galway, University Road, Galway, Ireland*
*3: School of Computer Science & Mathematics, Keele University, Staffordshire, United Kingdom*

In this study, the Deep Symbolic Optimization (DSO) algorithm is used to derive precise approximations for both the extension-force relationship of the Worm-Like Chain (WLC) model and a non-Gaussian probability distribution function for polymer chain length. The latter one is based on Kuhn and Gruen's non-Gaussian statistical theory [1]. Existing approximation methods in literature frequently yield complex equations that deviate from analytical solutions, thus limiting their practical utility. The objective of this work is to identify a set of simple yet accurate approximations that effectively characterize polymer extension models.

The proposed expressions for the WLC extension-force dependency achieve a very small relative error within the relevant variable range, enabling direct application to fit force-extension curves in molecular force spectroscopy experiments. A comparative analysis with recently suggested methods [2] reveals that the DSO-based approach surpasses traditional techniques in accuracy while preserving equation simplicity. Furthermore, we introduce novel approximations for the non-Gaussian probability distribution function of polymer chain length [3], expanding its applicability across a wider spectrum of chain segment numbers. This enhancement allows for more precise modeling of the behavior of polymers.

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**Assessing the Robustness of Data-Driven Impact Localization Models Under Real-World Experimental Variability**

von Cramon-Taubadel, Emanuel (1); Becker, Martin (2); Weißgraeber, Philipp (1) 14:40
*1: University Rostock, Germany*
*2: University Marburg, Germany*

Composites have greatly contributed to increased fuel efficiency in the aerospace sector by offering a high strength-to-weight ratio and tailorable mechanical properties. A challenge in their adoption is their susceptibility to impacts that leave little to no visible damage on the surface while still causing internal damage [1]. Structural health monitoring (SHM) promises to reduce the maintenance required to identify these damages through real-time impact monitoring. Common physics-based approaches triangulate the impact location by tracking the time of arrival (TOA) of the impact induced wave at various sensor locations [2], requiring highly accurate sensors and complex mechanical models. Using data-driven machine learning (ML), less accurate low-cost micro-electromechanical-systems (MEMS) accelerometers have shown high accuracy impact localization performance, even though they lack the resolution required for conventional TOA calculations [3]. Further evaluation of this novel approach requires more research into model robustness under real-world conditions such as changing boundary conditions or mechanical properties.
This study systematically examines the robustness of ML-based impact detection on a carbon-fiber–reinforced plastic (CFRP) plate with sparse MEMS sensors. Using an automated testbed, we collect over 500.000 real-world datapoints in diverse experiments. With this data, we train a proposed regression convolutional neural network (CNN) and compare its performance and robustness to a commonly used classification CNN. We also explore transfer learning (TL) for structural modifications by bonding a stiffener to the plates centerline and increasing its stiffness in three discrete levels. The regression model is robust towards small changes in the experimental setup, with its accuracy dropping less than 1%. It outperforms the classification variant with an improved accuracy of 1 to 5%. For larger physical changes, the performance significantly drops for both models, though the regression model retains an accuracy up to 33% higher than the classification model. Using TL for the stiffened plate configuration, we are able to reduce the amount of new training data by 88% while only reducing the localization accuracy by 2%.

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**Universal Design of Elastic Microstructures by Inverse Neural Networks**

Eidel, Bernhard; Neelakandan, Aagashram 15:00
*TU Freiberg, Germany*

Designing heterogeneous elastic materials to meet prescribed effective behavior is a central inverse problem: identify a feasible microstructure whose homogenized elasticity tensor matches a given target within specified tolerances. Here, the target effective tensor is provided together with the elastic parameters of the two constituent phases, which are equally prescribed inputs to the design task.

We present a differentiable learning pipeline that couples a frozen forward surrogate with an inverse neural network. The forward surrogate maps microstructural descriptors and the prescribed phase

elastic parameters to the effective elasticity tensor computed via first-order computational homogenization under periodic boundary conditions. Conditioned on the target tensor and the phase parameters, the inverse network proposes admissible microstructures, which are immediately validated by the forward surrogate within an end-to-end differentiable objective.

By training across a broad range of phase properties and elastic contrasts, the inverse model generalizes to almost arbitrary elastic phase parameters and their combinations, enabling "universal" microstructure design without retraining for new constituent materials.

**Data-Driven Surrogate Modeling for Long-Term Fatigue Load Prediction in Wind Energy Systems**

Albers, Hannes (1); Requate, Niklas (2); Wiens, Marcus (2); Othmane, Amine (3); Thomas, Philipp (2); Maaß, Peter (1); Flaßkamp, Kathrin (3)

*1: Universität Bremen, Germany*
*2: Fraunhofer IWES, Bremerhaven, Germany*
*3: Universität des Saarlandes, Saarbrücken, Germany*

15:20

High-fidelity numerical simulations play a central role in the analysis and lifetime assessment of wind-energy systems, particularly for the estimation of long-term fatigue loads. However, their high computational cost poses a significant challenge for large-scale studies, such as those required in turbine recertification and lifetime extension analyses. In this contribution, we explore the use of machine-learning–based surrogate models as an efficient alternative for the simulation of wind turbine dynamics.

Building on recent advances in neural operator learning, we investigate surrogate modeling approaches based on the Fourier Neural Operator (FNO) architecture, which is designed to represent complex spatiotemporal input–output relationships. The proposed models are trained on simulation data capturing a broad range of wind conditions and corresponding structural responses. Their performance is assessed through comparisons with established high-fidelity reference simulations, with particular emphasis on their applicability to fatigue-related quantities of interest.

The results highlight the potential of neural operator–based surrogate models to balance computational efficiency and predictive accuracy in the context of fatigue load estimation. This work aims to contribute to ongoing efforts toward scalable simulation frameworks for wind-energy applications and to stimulate discussion on the role of modern machine-learning methods in long-term structural assessment.

**Relating Stochastic Microstructural Geometric Imperfections to Effective Quantities' Uncertainty using Reduced Order Models and Machine Learning**

Chitnis, Tanmay (1); Fritzen, Felix (1); Massart, Thierry (2); Noels, Ludovic (3)

*1: Institute of Applied Mechanics – Data Analytics in Engineering, University of Stuttgart, Germany*
*2: BATir, Building, Architecture & Town Planning, Université Libre de Bruxelles (ULB), Belgium*
*3: Department of Aeronautics and Mechanical Engineering, Computational & Multiscale Mechanics of Materials, University of Liege, Belgium*

15:40

Additive manufacturing (AM) has emerged as a transformative method for fabricating materials with architecturally designed microstructures (MS). However, it inherently introduces stochastic geometric imperfections, such as surface waviness and local deviations, which significantly influence both the linear and nonlinear effective constitutive response of the final material [1]. Quantifying the uncertainty induced by these inevitable imperfections is the aim of this work. We propose a data-driven framework that leverages computationally efficient reduced-order models (ROMs) together with machine learning to predict distributions of effective responses (for example, stress fields and scalar stress measures) as functions of a compact and interpretable set of microstructural descriptors.

Methodologically, we construct a snapshot-based Proper Orthogonal Decomposition (POD)-based reduced-order model (ROM) from high-fidelity, full-field, small-strain solutions of a pristine, two-phase composite microstructure. These solutions are generated using our in-house FFT-based iterative solver FANS [2] operating on structured voxel meshes. To emulate realistic manufacturing noise,

we generate a portfolio of perturbed microstructures by modifying the inclusion level-set with a superposition of randomized three-dimensional Gaussian kernels. These perturbations mimic surface and geometric irregularities while explicitly constraining net volume-fraction deviations to within ±1% of the original design, ensuring physically plausible variants. The ROM, calibrated exclusively on the pristine geometry, is subsequently evaluated against this ensemble of perturbed variants to quantify the error in its predicted homogenized stress response under path-dependent $J_2$ plasticity.

To characterize the morphological perturbations in a compact, physically interpretable manner, we introduce a small set of geometric descriptors that are inexpensive to compute yet sensitive to the types of surface noise introduced. A Gaussian Process Regression (GPR) model is then employed to map these descriptors to the mean change in the quantity of interest (e.g., stress) and to its standard deviation, enabling probabilistic forecasts of bias and spread in the effective response. The resulting mapping provides a preliminary, scalable route for practical inverse design, where allowable manufacturing tolerances can be prescribed based on acceptable property variance. Future work will extend this framework to more complex microstructural topologies, finite-strain, rate-dependent constitutive models, and the development of enhanced, physically interpretable descriptors.

References:

[1] L. Liu, et al., “Elastic and failure response of imperfect three-dimensional metallic lattices: the role of geometric defects induced by Selective Laser Melting,” Journal of the Mechanics and Physics of Solids, vol. 107, pp. 160–184, 2017.

[2] Leuschner, M., et al., “Fourier-Accelerated Nodal Solvers (FANS) for homogenization problems,” Computational Mechanics, vol. 62, pp. 359–392, 2018.

## S25.08: Neural Operator Learning

Date: March 20, 2026 08:30–10:30
Room: KII, M17.01
Chair(s): Götschel, Sebastian

### Hard-constraining Boundary Conditions for Physics-Informed Neural Operators

Göschel, Niklas; Götschel, Sebastian; Ruprecht, Daniel 08:30
*Hamburg University of Technology, Germany*

Machine learning-based techniques, such as physics-informed neural networks and physics-informed neural operators, are increasingly effective at solving complex systems of partial differential equations. Boundary conditions in these models can be enforced weakly by penalizing deviations in the loss function or strongly by training a solution structure that inherently matches the prescribed values and derivatives. While the former approach is straightforward to implement, the latter can significantly enhance accuracy and reduce training times.
However, previous approaches to strongly enforcing Neumann or Robin boundary conditions require a domain with a fully $C^1$ boundary and, as we demonstrate, can lead to instability if those boundary conditions are posed on a segment of the boundary that is piecewise $C^1$ but only $C^0$ globally. We introduce a generalization of the approach by Sukumar & Srivastava (https://doi.org/10.1016/j.cma.2021.114333) and a new approach based on orthogonal projections that overcome this limitation. The performance of these new techniques is compared against weakly and semi-weakly enforced boundary conditions for the scalar Darcy flow equation and the stationary Navier-Stokes equations.

**Neural Operators for Accelerating Iterative Solvers**

Eshaghi Khanghah, Mohammad Sadegh (1); Zhuang, Xiaoying (1); Rabczuk, Timon (2)

*1: Leibniz Univeristy Hannover, Germany*
*2: Bauhaus Univeristy Weimar, Germany*

08:50

High-fidelity simulation of partial differential equations (PDEs) is central to modeling complex physical and engineering systems, yet it remains computationally expensive when addressing high-dimensional domains, stiff dynamics, or many-query settings involving varying parameters, initial conditions, or boundary data. Neural operators have emerged as a promising paradigm by learning mappings between function spaces, but existing approaches face key challenges in enforcing physical consistency, handling long-time dynamics, and ensuring reliability beyond the training distribution.

In this talk, we present a unified perspective on recent advances in physics-informed and hybrid neural operator methodologies that address these challenges from complementary angles. First, we introduce the Variational Physics-Informed Neural Operator (VINO), which embeds PDEs through their variational (energy) formulations. By minimizing the energy functional over discretized elements, VINO eliminates the need for labeled data, enables efficient loss evaluation, and achieves improved accuracy and scalability compared to both standard physics-informed neural operators and classical solvers, particularly at increasing mesh resolutions.

We then focus on time-dependent and interfacial PDEs through the Multi-Head Neural Operator (MHNO), a novel architecture designed to overcome error accumulation and temporal inefficiency in existing neural operators. MHNO employs time-step-specific projections and explicit temporal connections inspired by message passing, allowing all time steps to be predicted in a single forward pass while capturing long-term dependencies. Applications to a range of phase-field and interfacial dynamics problems demonstrate superior accuracy, efficiency, and scalability.

Finally, we introduce Neural Operator Warm Starts (NOWS), a hybrid framework that bridges learned neural operators with classical iterative solvers. By providing high-quality initial guesses for Krylov methods, NOWS significantly reduces iteration counts and end-to-end runtimes—by up to 90%—while preserving the robustness and convergence guarantees of traditional numerical methods.

Together, these works illustrate a cohesive strategy for integrating physical structure, architectural innovations, and hybrid learning–numerics into neural operators, offering reliable, scalable, and efficient tools for next-generation PDE simulation across science and engineering.

**A physics-encoded Fourier neural operator approach for surrogate modeling of divergence-free stress fields in solids**

Khorrami, Mohammad S (2); Mianroodi, Jaber R (2); Goyal, Pawan (1); Oexle, David (1); Motahari, Soroush (2); Svendsen, Bob (2,3); Benner, Peter (1); Raabe, Dierk (2)

*1: Computational Methods in Systems and Control Theory, Max-Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany*
*2: Material Mechanics, RWTH Aachen University, Aachen, Germany*
*3: Microstructure Physics and Alloy Design, Max-Planck Institute for Sustainable Materials, Du ̈sseldorf, Germany*

09:10

The purpose of the current work is the development of a so-called physics-encoded Fourier neural operator (PeFNO) for surrogate modeling of the quasi-static equilibrium stress field in solids. Rather than accounting for constraints from physics in the loss function as done in the (now standard) physics-informed approach, the physics-encoded approach incorporates or ”encodes” such constraints directly into the network or operator architecture. As a result, in contrast to the physics-informed approach in which only training is physically constrained, both training and output are physically constrained in the physics-

encoded approach. For the current constraint of divergence-free stress, a novel encoding approach based
on a stress potential is proposed. As a "proof-of-concept" example application of the proposed PeFNO, a heterogeneous polycrystalline material consisting of isotropic elastic grains subject to uniaxial extension
is considered. Stress field data for training are obtained from the numerical solution of a corresponding
boundary-value problem for quasi-static mechanical equilibrium. This data is also employed to train an
analogous physics-guided FNO (PgFNO), where the underlying physics is only captured in the data and
not in the networks architecture, and a physics-informed FNO (PiFNO) for comparison. As confirmed by this comparison and as expected on the basis of their differences, the output of the trained PeFNO is significantly more accurate in satisfying mechanical equilibrium than the output of either the trained PgFNO or the trained PiFNO.

**Neural Operator Modeling of History-Dependent Plastic Deformation in Heterogeneous Media**

Sunil Umate, Kartik (1); Taghikhani, Kianoosh (2); Motahari, Soroush (1); Najian Asl, Reza (2); Apel, Markus (2); Roters, Franz (1); Liu, Chuanlai (1); Raabe, Dierk (1); Rezaei, Shahed (2)
*1: ACCESS e.V., Germany*
*2: Max Planck Institute for Sustainable Materials*

09:30

Neural operators have recently emerged as powerful surrogate models for learning solution operators of partial differential equations, yet their applicability to full-field, history-dependent crystal plasticity simulations remains insufficiently explored. We perform a systematic comparison of different neural operator architectures, including Fourier Neural Operators (FNO), Convolutional Neural Operators (CNO), and Conditional Neural Fields (CNF). Different temporal learning strategies are examined, including autoregressive time stepping and direct full-trajectory prediction, and are evaluated with respect to accuracy, long-time stability, and computational cost. The models are evaluated on microstructures with unseen textures and grain-size distributions, as well as outside the training domain in terms of higher deformation levels and increased spatial resolution, showing robust predictive performance. Our results highlight the strengths and limitations of each architecture and training strategy for highly nonlinear, history-dependent material behavior. To foster reproducibility and further research, all datasets, reference solutions, and evaluation protocols will be made publicly available, establishing a benchmark for neural-operator-based modeling of plasticity in heterogeneous microstructures.

**A Surrogate Model for Structure-Property Linkages in Polycrystals Using Physics-Informed Neural Operators**

Awad, Ahmad; Scheunemann, Lisa
*Institute of Applied Mechanics, RWTH Aachen University, Germany*

09:50

Austenitic stainless steels represent over 50% of the global stainless-steel consumption and remain essential due to their broad industrial applicability [1]. Sustainable production therefore requires efficient recycling routes that allow the reuse of materials without degrading mechanical performance.

Despite generally reliable sorting technologies, scrap-based feedstock can show small but non-negligible compositional variations. Such deviations are particularly critical for metastable austenitic stainless steels, which are governed by deformation-induced martensitic transformation. The austenite-to-martensite transformation is highly sensitive to the chemical composition. Slight variations in elements such as Ni and Cr alter austenite stability, stacking fault energy, and consequently the amount of martensite formed during deformation [2]. These microstructural changes directly influence the macroscopic mechanical behavior.

The objective of this contribution is to describe the above-mentioned behavior through a forward (micro)structure–property linkage via a surrogate model based on neural networks (NNs) and Physics-Informed Neural Operators (PINOs) [3]. The model shall capture the microstructural distribution of austenite and martensite, and link the multiphase microstructure to the resulting elastoplastic mechanical response. This framework establishes a fast alternative to classical physics-based modeling approaches for structure-property linkages.

[1] T. Trzepieciński and S. M. Najm, 2024. Current Trends in Metallic Materials for Body Panels and Structural Members Used in the Automotive Industry. Materials. https://doi.org/10.3390/ma17030590.

[2] T. Liu, S. Mukhopadhyay, C. Li, T. Li, Y. Ren, P. Singh, A. Devaraj, 2025. The impact of nickel concentration and stacking fault energy on deformation mechanisms in high-purity austenitic Fe-Cr-Ni alloys. Materials Characterization. https://doi.org/10.1016/j.matchar.2025.115046.

[3] Z. Li, H. Zheng, N. Kovachki, D. Jin, H. Chen, B. Liu, K. Azizzadenesheli, A. Anandkumar, 2024. Physics-Informed Neural Operator for Learning Partial Differential Equations. ACM / IMS J. Data Sci. https://doi.org/10.1145/3648506.

**Accelerating Conjugate Gradient Solvers for Homogenization Problems with Unitary Neural Operators**

Herb, Julius; Fritzen, Felix 10:10
*Institute of Applied Mechanics, University of Stuttgart, Germany*

Accurate and efficient solvers for parametric partial differential equations (PDEs) play a central role in computational mechanics, especially in applications involving composites and architectured materials. Designing such materials and predicting their behavior in practical applications requires solving a large number of homogenization problems for varying microstructures and material parameters. While classical numerical solvers offer reliable and accurate solutions supported by a solid theoretical foundation, their high computational costs and slow convergence remain limiting factors. In recent years, neural operators [1] are emerging as a powerful tool for predicting the solution of parametric PDEs. However, purely data-driven surrogate models typically lack accuracy guarantees. This motivates the development of hybrid approaches that retain the convergence guarantees of classical algorithms while exploiting data-driven components to improve efficiency.

In this talk, we present UNO-CG [2], a hybrid solver that accelerates the Conjugate Gradient method by incorporating Unitary Neural Operators (UNOs) as machine-learned preconditioners. UNOs are a modification of Fourier Neural Operators [3] and specifically designed to be admissible within CG, i.e., maintaining guaranteed solver convergence. They can be interpreted as learning numerical Green's functions, providing a data-driven analogue to expert-designed preconditioners such as Fourier-accelerated methods [4, 5], yet applicable beyond periodic boundary conditions to which FFT-based solvers are usually restricted. We demonstrate the performance of UNO-CG on large-scale homogenization problems. Our results show a substantial reduction in CG iterations and competitive performance compared to expert-designed preconditioners. In addition, we discuss efficient training strategies requiring only few data samples and outline extensions of the approach to further problem formulations.

[1] N. Kovachki, Z. Li, B. Liu, et al. [2023]: "Neural operator: learning maps between function spaces with applications to PDEs", J. Mach. Learn. Res.
[2] J. Herb, F. Fritzen [2025]: "Accelerating Conjugate Gradient Solvers for Homogenization Problems with Unitary Neural Operators", arXiv.
[3] Z. Li, N. Kovachki, K. Azizzadenesheli, et al. [2021]: "Fourier Neural Operator for Parametric Partial Differential Equations", ICLR 2021.
[4] M. Leuschner M, F. Fritzen [2018]: "Fourier-Accelerated Nodal Solvers (FANS) for homogenization problems", Computational Mechanics 62(3)
[5] M. Schneider, D. Merkert, M. Kabel [2017]: "FFT-based homogenization for microstructures discretized by linear hexahedral elements", IJNME 109(10)

## S26: Modeling, analysis and simulation of molecular systems

Organizer(s): Hassan, Muhammad *(Technische Universität München)*
Stamm, Benjamin *(University of Stuttgart)*

## S26.01: Complex materials and environment

Date: March 17, 2026 08:30–10:30
Room: KI, M11.62
Chair(s): Stamm, Benjamin

### Automatic identification equivalent atoms in complex materials and molecules

Lai, King Chun; Matera, Sebastian; Scheurer, Christoph; Reuter, Karsten 08:30
*Fritz Haber Institute of the MPS, Germany*

Classification of local atomic environments (LAEs) is an inevitable task in most atomic-scale modeling and simulation. The reason is trivial, atoms' characteristics are predominantly determined by neighbors within a limited radius. The task itself, however, is abstract and error-prone due to the diversity of structures and the often ambiguous relationship between geometry and atomic behaviors. To address these issues, we have developed the Descriptor Embedding and Clustering for Atomisitic-environment Framework (DECAF) during the last years [1]. DECAF automatically identifies equivalence groups within atomic structure datasets on the basis of the LAEs. To achieve this, DECAF proceeds in three steps: i) a mapping of the LAE of each atom in the dataset onto a point in a high-dimensional vector space automatically exploiting fundamantal physical symmetries, ii) dimension-reduction using Multidimensional Scaling, and iii) Mean Shift Clustering to obtain the equivalence groups. We showcase DECAF on a set of nanotructures and provide examples where this has been exploited such as automatic process exploration [2] or active learning.
[1] Lai, K. C., et al. J. Chem. Phys. 159.2 (2023).
[2] Lai, K. C., et al. Phys. Rev. Lett. 134.9 (2025): 096201.

### Deformation of molecular systems using a dynamical reduced basis approach in combination with empirical interpolation to efficiently evaluate force fields

Reihn, Maximilian 08:50
*University Stuttgart, Germany*

The athermal quasistatic deformation method provides an elegant solution to overcome the limitation of short time steps in molecular dynamics simulations. It provides overdamped conditions, allowing for the extraction of purely structural responses in the absence of thermal vibration. However, it requires computationally expensive sequences of affine deformation followed by minimization of the potential energy to incrementally find the path in the potential energy landscape that corresponds to the correct solution trajectory. To mitigate this computational bottleneck, we propose an adaptive Reduced Order Model (ROM) framework that accelerates energy minimization by projecting the system behavious onto a low-dimensional subspace. Unlike traditional offline-online reduction strategies that often fail to capture the chaotic, spatially localized plasticity of disordered system - our approach constructs the reduced basis dynamically. We employ the Empirical Interpolation Method (EIM) to reconstruct the global force field from a subset of atomic interactions, chosen by a greedy strategy, to significantly reduce the cost of force evaluations. Crucially, the basis is incrementally enriched via updates whenever the approximation residual exceeds a tolerance. This ensures that the reduced subspace dynamically evolves to capture emerging Shear Transformation Zones (STZs) without a priori knowledge of their location. We demonstrate that this online adaptive strategy maintains high fidelity to the true AQS trajectory while effectively decoupling the computational complexity from the total system size.

**Generative AI for disordered Materials**

Bachhav, Bhagyashri; Markert, Bernd; Bamer, Franz
*RWTH Aachen University, Germany*

09:10

Network structures in glass materials are crucial for understanding the glass transition, surface phenomena, advancing applications in nanotechnology and materials science, and structural engineering in general. Intriguingly, some molecular models can be generated based on real images of two-dimensional silica structure obtained by Lichtenstein et al. [1,2]. However, generating physically meaningful amorphous 2D network structures remains challenging due to the stringent requirements on local coordination, ring-size statistics, and long-range topological correlations. These are difficult to satisfy using conventional melt–quench molecular dynamics alone. Furthermore, generating samples is computationally expensive, as shown in Bachhav et al. [3]. To overcome this issue, we present a novel and robust GAN framework for generating structurally realistic 2D silica glass networks that accurately reproduce the silica glass observed experimentally by Lichtenstein. GANs can learn the underlying distribution of the silica network and its variations, leading to near-exact sample generation. The proposed network is trained on data obtained from dual Monte Carlo bond switching algorithm, as described in Bachhav et al.[3]. The goal of this contribution is to understand the ability of the GAN to generate physically admissible synthetic samples of silica glass, implicitly incorporating the topological constraints of molecular network structures.

References:

[1] Lichtenstein, Leonid, Markus Heyde, and Hans-Joachim Freund. "Crystalline-vitreous interface in two dimensional silica." Physical Review Letters 109.10 (2012): 106101.

[2] Bamer, Franz, et al. "Molecular mechanics of disordered solids." Archives of Computational Methods in Engineering 30.3 (2023): 2105-2180.

[3] Bachhav, Bhagyashri, et al. "Predicting fracture in disordered network materials using the local intelligent stress threshold indicator." Communications Physics 8.1 (2025): 369.

**Efficient generation and explicit dimensionality of Lie group-equivariant and permutation-invariant bases**

Zhang, Liwei
*RWTH Aachen University*

09:30

Most of the physical properties of interest that arose in molecular simulations exhibited certain symmetries, including Permutation Invariance(PI) and Lie Group Equivariance (GE). In this presentation, we propose a practical construction of GE and PI multi-variable functions from the knowledge of a basis that is stable with respect to the group action. In particular, the construction requires neither the knowledge of Clebsch–Gordan coefficients nor the looping over the permutations of variables. For specific groups such as SO(3) and SU (2), it also allows us to compute the exact dimension of the group-equivariant and permutation-invariant basis explicitly. We also present numerical simulations to show that the proposed method scales polynomially instead of exponentially for existing methods in the literature.

**A General and Minimally Empirical Implicit Solvation Model from First Principles**

Wittmann, Lukas; Grimme, Stefan
*Mulliken Center for Theoretical Chemistry, Beringstraße 4, 53115 Bonn, Germany*

09:50

We present GEMS, a general and minimally empirical implicit solvation model derived from first principles. GEMS builds on the conductor-like polarizable continuum model but replaces the typically static cavity with a novel, molecule- and atom-specific one [1], defined by a smooth, fully differentiable solvent-excluded-surface-like representation. This forms the foundation for all components: dispersion is described by a true continuum-integrated model derived from DFT-D4 – explicitly taking into account the cavity shape; short-range solute-solvent repulsion is treated self-consistently; and a novel cavitation term is derived using statistical mechanics. GEMS further accounts for the solute's

loss of translational and rotational entropy upon transfer to solution, as well as for the energetic change associated with solvent-mediated charge transfer.

Despite its theoretical sophistication, GEMS remains fully differentiable [2], enabling both efficient geometry optimizations and Hessian calculations. The model runs at a cost comparable to SMD or COSMO-RS, is compatible with most electronic-structure methods, and is easily applicable: it requires only the solvent geometry, permittivity, and density. The physical basis of GEMS allows us to use only a few global parameters. Nonetheless, parameterizing and validating the model still requires large and diverse datasets – something that is not sufficiently available for solvation models. To overcome this, we compiled a dataset with over 15,000 experimental data points [3] – such as solvation free energies, partition coefficients, and acid dissociation constants. On these sets, GEMS matches the accuracy of SMD and COSMO-RS for simple neutral organic molecules while showing improved robustness and accuracy for more challenging cases such as (zwitter)ions or acid dissociation constants.

The model will be available in ORCA and in our modular, open-source solvation toolbox library.

[1] C. Plett, M. Stahn, M. Bursch, J.-M. Mewes and S. Grimme, *J. Phys. Chem. Lett.*, 2024, **15**, 2462-2469.

[2] L. Wittmann, M. Garcia-Ratés and C. Riplinger, *J. Comput. Chem.*, 2025, **46**, DOI: 10.1002/jcc.70099.

[3] L. Wittmann, C. S. Selzer and S. Grimme, *Chem. Sci.*, 2025, DOI: 10.1039/D5SC06406F.

**Accurate continuum solvation for fast semi-empirical methods**

Dahl, Robin; Wittmann, Lukas; Froitzheim, Thomas; Grimme, Stefan 10:10
*Universität Bonn, Mulliken Center for Theoretical Chemistry, Bonn, Germany*

Capturing solvation effects is essential for realistic quantum-chemical modeling. Recent advances in semiempirical electronic structure methods—most notably g-xTB—provide a powerful foundation for large-scale solvation treatments, offering near-DFT accuracy at tight-binding cost and enabling reliable solvation contributions even for large (bio)molecules.

In this contribution, we present the developments towards a next-generation continuum solvation model specifically tailored to, and parameterized for, g-xTB, with the aim of delivering fast but accurate solvation free energies to preserve the efficiency of tight-binding approaches. The framework combines a polarizable continuum description of electrostatics with non-electrostatic contributions accounting for cavitation, hydrogen bonding, dispersion, and related effects. A central development is the refinement of the solute electronic description beyond the conventional monopole approximation, advancing toward a multipole representation derived from Mulliken populations that more faithfully reflects the underlying quantum density. These improvements are investigated within the linear-scaling domain-decomposition conductor-like screening model (ddCOSMO) as well as the efficient analytical linearized Poisson–Boltzmann (ALPB) formalism.

A further focus is the construction of the molecular cavity through environment-responsive radii scaling. By parameterizing a scaling function based on effective solute–solvent interactions—made explicit, for example, via charge-dependent terms—we obtain chemically more appropriate cavity radii than standard gas-phase van der Waals values. Because COSMO-type models depend strongly on the cavity definition, this strategy can substantially improve solvation free energies. In addition, it can serve as a starting point for an improved Born integrator in the ALPB formalism, thereby making the computation of suitable Born radii more chemically meaningful compared to a purely volumetric integration.

Furthermore, we discuss the theoretical formulation, the supporting open-source software infrastructure, and demonstrate accuracy, scalability, and performance as a function of molecular size.

**S26.02: Sampling of molecular systems**

Date: March 17, 2026 16:30–18:30
Room: KI, M11.62
Chair(s): Ehrlacher, Virginie

**Estimating Finite-Size Effects in Molecular Simulations**

Reible, Benedikt (1); Hartmann, Carsten (2); Delle Site, Luigi (1)
*1: Freie Universität Berlin*
*2: Brandenburgische Technische Universität Cottbus-Senftenberg*

16:30

Determining an appropriate simulation-box size is a central challenge in molecular simulations: it should be large enough to provide a physically consistent representation of the system, yet small enough to remain computationally efficient. This problem is known under the name of finite-size effects, and several criteria have been adopted in order to determine their relevance in specific situations. In this talk, I present a rigorous approach to this problem based on the two-sided Bogoliubov inequality for classical and quantum many-body systems. This inequality provides tight bounds on the free-energy cost of partitioning a system into independent subsystems, and it naturally leads to a quality factor that quantifies the statistical-mechanical consistency achieved by a chosen box size. For systems with two-body interactions and a known radial distribution function, this quality factor can be computed efficiently from six-dimensional integrals, providing a first-principles criterion for estimating finite-size effects, without the need of running any simulation.

**The narrow escape problem**

Carillo, Louis; Lelièvre, Tony; Stoltz, Gabriel; Vaes, Urbain
*CERMICS, France*

16:50

The narrow escape problem is a prototypical example to study entropic metastability, inspired by concrete applications in biology and chemistry. The problem is the determination of the exit time and position of a Brownian particle trapped in a domain with narrow holes. Unlike the usual double well potential, this form of metastability is not of energetic form as there is no potential involved, hence no Eyring-Kramers formula. Our goal is to study this problem in any dimension for arbitrary shapes of hole, and thanks to the quasi-stationary distribution approach to metastability, to rigorously derive the counterpart Eyring-Kramers type formulas in this context. Our numerical predictions are illustrated by numerical simulations, both Monte Carlo like and determinstic ones based on solving appropriate partial differential equations.

**Sampling equilibrium states via normalizing flow approximation of transport maps**

Rehman, Zia Ur; Friesecke, Gero
*Technical University of Munich, Germany*

17:10

In a celebrated paper [NOKW19], No´e and coworkers introduced an efficient method for sampling high-dimensional Boltzmann distributions arising in molecular dynamics via normalizing flow approximation of transport maps. Here, we place this approach on a firm mathematical foundation. We show that smooth transport maps connecting a reference measure to the target Boltzmann distribution can be approximated strongly in L1 by ReLU neural networks and by invertible normalizing flows such as RealNVP. This ensures that the generated densities converge to the true equilibrium distributions, even in the presence of singular molecular potentials. Our analysis provides a rigorous link between classical transport theory and modern deep generative modeling, offering a constructive framework for flow-based Boltzmann sampling. Numerical illustrations on alanine dipeptide and Langevin systems demonstrate that flow-based models can capture key features of equilibrium distributions and metastable dynamics, confirming the practical relevance of the theoretical results for sampling in high-dimensional molecular systems.

**Entropic Transfer Operators**

Stier, Thilo D.
*Georg August University Göttingen, Germany*

17:30

Entropic transfer operators (ETO) are a way to estimate the transfer operator of a dynamical system. This can be used as a tool to generate meaninful low dimensional embeddings of the data as well as analyzing properties like cyclicity, (meta-) stability and transition paths of the system.

The underlying principle of ETO is similar to Ulam's method in that it aggregates data in spatial neighborhoods to estimate the transition distribution, but it differs in that it does not use a fixed partition of space, instead making use of the favourable properties of entropic optimal (self-) transport kernels to smoothly combine all observed transtitions to make a global estimate of the transfer operator. This has several advantages including having fewer hyperparameters and automatically adapting to the intrinsic dimension of the data, at the cost of higher computational effort.

The talk shows the basic working principle of ETO and preliminary applications to conformational analysis of molecules.

**An O(logN) Kinetic Monte Carlo Algorithm for Transport Simulation with Long-Range Interactions**

Bat-Erdene, Bat-Amgalan; Ebrahimi Viand, Roya; Reuter, Karsten; Matera, Sebastian 17:50
*Fritz Haber Institute, Germany*

Ion diffusion in solids is characterized by rare events, where ions jump between sites on the crystal lattice. These dynamics can be coarse-grained to Markov jump processes and simulated using kinetic Monte Carlo (kMC) methods. However, a characteristic of charge transport is the presence of long-range Coulomb interactions. Even when utilizing optimized iterative formulas for transition rates, the global nature of these interactions causes a complexity of O($N$) in the system size $N$. In contrast, kMC with only short-range interactions can be made to scale as O(log$N$) per step by restricting updates to local rates and employing tree based algorithms for event selection and time increment calculation. Thus, Coulomb interactions cause a significant computational overhead. We address this issue by a novel time discretization approach inspired by the tau-leaping method. Starting with exact values for the rates, the approach conducts fast incremental updates O(log$N$) in every step based on a truncated short-range potential. Inevitably, this leads to a deviation of the rates from their true values as simulation proceeds. Therefore, a full recalculation of the rates is conducted once every O($N$) steps, which can be done in O($N$log$N$) using Fast Fourier Transform resulting in an average cost of O(log$N$) per step. We demonstrate the scheme for charge transport on a cubic lattice using our in-house kMC framework. Special emphasis is placed on the balance between discretization error and efficiency, as well as the influence of the truncation radius on both.

## S26.03: Numerical analysis (Eigenvalue problems)

Date: March 18, 2026 08:30–09:30
Room: KI, M11.62
Chair(s): Lasser, Caroline

**Metric-based nonlinear model order reduction with applications to quantum chemistry**

Dusson, Geneviève 08:30
*CNRS and Université Marie et Louis Pasteur, France*

A broad class of problems in science and engineering involves the repeated solution of partial differential equations (PDEs) for different parameter values. Linear reduced order models are a powerful tool to decrease the computational cost of these simulations by approximating the solutions in a low-dimensional space. They have proven highly effective in many settings; however, they often perform poorly for transport-dominated PDEs, where key solution features such as translations cannot be accurately represented in a linear subspace.

To overcome these limitations, several nonlinear reduced order models have recently been proposed, including approaches based on quadratic or polynomial mappings and neural networks. In this talk, I will present an alternative metric-based approach to nonlinear model order reduction. The central idea is to replace linear combinations in low-dimensional spaces with barycenters taken with respect to a suitably chosen metric, computed from a small number of representative solutions. In particular, I will provide constructions based on the Wasserstein distance from optimal transport, which is well

adapted to capturing translations. I will also show how the choice of metric can be adapted to incorporate physical constraints, such as sparsity or prescribed marginals. The proposed methodology will be illustrated through numerical examples involving the approximation of electronic densities and pair densities arising in quantum chemistry.

**Model Order Reduction for Parametric Hermitian Eigenvalue Problems: Local Acceleration with Taylor-Reduced Basis Method**

Stamm, Benjamin; Zeng, Zhuoyao
*University of Stuttgart, Germany*

09:10

The Taylor Reduced Basis Method (Taylor-RBM) is a classical approach in model order reduction for parametric problems. By augmenting the basis with derivatives of the solution at a reference parameter point, Taylor-RBM accelerates the convergence of Galerkin projections for nearby parameter values. This work extends the Taylor-RBM framework to parametric linear Hermitian eigenvalue problems on uni- and multivariate parameter spaces. We follow the methodology based on analytic perturbation theory to handle the total projector of isolated eigenvalues, ensuring a robust representation of the eigenspace and of the eigenvalue sum. In addition to a concise theoretical convergence analysis, we discuss practical implementation aspects of the method.

## S26.04: High Performance Algorithms

Date: March 18, 2026 14:00–16:00
Room: KI, M11.62
Chair(s): Lipparini, Filippo

**Breaking the exascale barrier for the electronic structure problem in ab-initio molecular dynamics**

Kühne, Thomas
*CASUS/HZDR, Germany*

14:00

The non-orthogonal local submatrix method applied to electronic structure–based molecular dynamics simulations is shown to exceed 1.1 EFLOP/s in FP16/FP32-mixed floating-point arithmetic when using 4400 NVIDIA A100 GPUs of the Perlmutter system. This is enabled by a modification of the original method that pushes the sustained fraction of the peak performance to about 80%. Example calculations are performed for SARS-CoV-2 spike proteins with up to 83 million atoms.

**Algorithmic differentiation for plane-wave DFT: materials design, error control and learning model parameters**

Herbst, Michael (1,2); Schmitz, Niklas (1,2); Ploumhans, Bruno (1,2)
*1: Mathematics for Materials Modelling (MatMat), Institute of Mathematics & Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*
*2: National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*

14:20

Reliable algorithmic differentiation techniques offer great promise for the inverse design of materials, improved density-functional theory (DFT) models or the propagation of uncertainties in first-principle modelling: three topics of current interest with direct consequences to improve accuracy and reliability of materials simulations. In recent work [1] we equipped the density-functional toolkit (DFTK, https://dftk.org) — our in-house Julia-based DFT code — with algorithmic differentiation capabilities. I will present some of the required algorithmic developments to robustly solve the arising linear response equations and discuss the perspectives of this framework following examples such as the inverse design of a semiconductor band gap, the learning of exchange-correlation functional parameters, or the propagation of DFT parameter uncertainties to relaxed structures.

[1] N. F. Schmitz, B. Ploumhans and M. F. Herbst. npj Computational Materials (2025). DOI 10.1038/s41524-025-01880-3

**Data-Driven Spectral Prediction for Accelerating Large-Scale Electronic Structure Calculations**

Ramirez-Hidalgo, Gustavo (1); Di Napoli, Edoardo (1); Genovese, Luigi (2); Davidovic, Davor (3); Wu, Xinzhe (1); Badrinarayanan, Abhiram (4); Novak, Jurica (3)

*1: Forschungszentrum Jülich, Germany*
*2: CEA / IRIG / MEM / $L_{\mathrm{Sim}}$*
*3: Ruđer Bošković Institute*
*4: University of Jyväskylä*

14:40

Solving large-scale sparse eigenproblems remains a significant computational bottleneck in materials science, particularly within Density Functional Theory (DFT) simulations on exascale architectures. This contribution presents the outcomes of LimitX, a project supported the EuroHPC-funded Inno4Scale framework. In LimitX we introduce a machine learning (ML) framework designed to predict spectral properties and accelerate the convergence of self-consistent field (SCF) cycles. To support this data-driven approach, we generated a comprehensive database comprising Hamiltonian and Overlap matrices derived from linear-scaling BigDFT simulations of 660 protein-protein complexes, ranging from 1,000 to 15,000 atoms. To address the dimensionality challenge of predicting full eigenspectra, we developed a methodology that predicts the coefficients of Chebyshev polynomials interpolating the spectrum, rather than individual eigenvalues. This transformation simplifies the learning task into a fixed-length vector prediction, ensuring scalability regardless of system size. We benchmarked three predictor models: Kernel Ridge Regression (KRR) with randomized spectral compression, Graph Neural Networks (GNN) adapted from SchNet, and Random Forests based on weighted Radial Distribution Functions (RDFs). All models utilize a fragment-based representation (amino acids) to reduce complexity while preserving structural relationships. The resulting models successfully predict the Density of States (DoS) with high fidelity. Additionally, the predicted spectra benefit rational filter eigensolvers by enabling more balanced workload distribution via the approximate DoS and by facilitating the construction of shifted polynomial preconditioners for solving the multi-shifts linear systems. By integrating these ML-driven priors, we provide a pathway to significantly reduce the computational cost of quantum simulations for complex biological systems.

**CDFCI: High-Performance Parallel Software for Large-Scale Many-Body Eigenvalue Problems**

Zhang, Yuejia

*Fudan University, China, People's Republic of*

15:00

We present CDFCI, a high-performance shared-memory parallel software package for computing low-lying eigenpairs of large-scale, non-relativistic fermionic Hamiltonians, arising in electronic structure and condensed matter simulations. CDFCI utilises a coordinate-descent-based selected configuration interaction (CI) approach, while leveraging dynamic task scheduling to achieve efficient workload distribution on modern multi-core CPU architectures. Numerical experiments on representative ab-initio electronic Hamiltonians and lattice models demonstrate state-of-the-art numerical accuracy, near-linear strong scaling up to 256 cores, and competitive performance when compared with existing selected CI and DMRG implementations. The software is open-source, well documented, and provides a Python interface facilitating integration into workflows such as PySCF. This is joint work with Zhe Wang, Jianfeng Lu, and Yingzhou Li.

**DiagLib: an Open-Source, Matrix-Free, Iterative Eigensolver**

Nottoli, Tommaso (1); Giannì, Ivan (1); Alessandro, Riccardo (2); Bröcker, Felix (3); Cianchino, Davide (4); Lapi, Lorenzo (1); Pes, Federica (5); Levitt, Antoine (6); Lipparini, Filippo (1)

*1: Università di Pisa, Italy*
*2: Università degli Studi di Perugia, Italy*
*3: RWTH Aachen University, Germany*
*4: Universität des Saarlandes, Germany*
*5: Università degli Studi di Cagliari, Italy*
*6: Université Paris-Saclay, France*

15:20

Quantum-chemical calculations often require computing for a small subset of eigenvalues and eigenvectors of very large matrices. In such cases, efficient dense solvers such as LAPACK cannot be used, and one must rely on iterative methods. These numerical solvers must be sufficiently robust to converge even in pathological situations, whether arising from the intrinsic difficulty of the quantum-chemical model, accidental complexities of specific molecular systems, or the use of diffuse basis sets.

We have recently developed DiagLib [1], an open-source Fortran library, which is designed for seamless integration into existing software. DiagLib offers the possibility of solving standard (including non-symmetric) and generalized eigenvalue problems, linear systems, and also the generalized eigenvalue problem encountered in linear response complete active space self-consisted field (LR-CASSCF) theory. In this contribution, we show its main functionalities through two representative large-scale quantum-chemical applications: the solution of the eigenvalue problem in the context of full configuration interaction (full-CI), and the solution of the generalized eigenvalue problem in LR-CASSCF [2].

For the former, DiagLib supports both the standard Davidson procedure and the more memory-efficient one given by the so-called locally optimal block preconditioned conjugate gradient (LOBPCG) method [3]. For the latter, metric-orthogonal expansion vectors are used to simplify the structure of the problem within the reduced subspace, yielding an eigenvalue problem of half the original size. In general, all solvers employ numerically stable and robust orthogonalization routines that produce vectors orthogonal to a given set – and mutually orthogonal – up to machine precision. The implementation uses a cost-effective Cholesky decomposition with iterative refinement to control the condition number, ensuring it remains no worse than the one carried by the original problem. These orthogonalization routines are exposed through the interface and can also be used as primitive components in other contexts.

We illustrate the stability and performance of the algorithms on real chemical systems, seeking up to hundreds of eigenvalues.

[1] See https://github.com/Molecolab-Pisa/diaglib (Last accessed: Jan 7th, 2026).

[2] R. Alessandro, I. Giannì, F. Pes, T. Nottoli, F. Lipparini, *J. Chem. Theory Comput.* **19**, 9025–9031 (2023).

[3] T. Nottoli, I. Giannì, A. Levitt, F. Lipparini, *Theo. Chem. Acc.* **142**, 69 (2023).

## S26.05: Density Functional Theory

Date: March 18, 2026 16:30–18:30
Room: KI, M11.62
Chair(s): Friesecke, Gero

**DFT and effective models for moiré materials**

CANCES, Eric

*Ecole des Ponts - Institut Polytechnique de Paris and Inria, France*

16:30

The design of multilayer 2D and moiré materials with specific electronic, optical, and mechanical properties is a relatively new, and very hot topic in condensed-matter physics and materials science.

I will discuss the theoretical foundation of Density-Functional Theory models for moiré materials. I will then explain how effective models at the moiré scale of Bistritzer-MacDonald type can be derived rigorously from Kohn-Sham Hamiltonians. If time allows, I will address some numerical issues.

This presentation will summarize a series of works with different collaborators (Louis Garrigue and David Gontier; Daniel Massatt, Long Meng, Etienne Polack and Xue Quan; Francis Nier; David Gontier and Solal Perrin-Roussel).

**A quantitative Hohenberg-Kohn theorem and the unexpected regularity of DFT for spinless fermions in one spatial dimension**

Carvalho Corso, Thiago (1); Laestadius, Andre (2) 16:50

*1: University of Stuttgart, Germany*
*2: Oslo Metropolitan University, Norway*

In this talk, we present some recent results on the existence and regularity of the (Kohn-Sham) density-to-potential map in the case of spinless fermions in one spatial dimension. More precisely, we start by recalling a complete characterization of $v$-representability obtained by the author in [1,2]. This result guarantes the existence of a bijective density-to-potential map for both interacting and non-interacting systems. We then focus on the regularity of this map as a function of the density and the coupling constant in front of the interaction term. More precisely, we first present a quantitative version of the Hohenberg-Kohn theorem, thereby showing that this map is Lipschitz continuous with respect to the natural Sobolev norms in the space of densities and potentials. In particular, this implies that the inverse (Kohn-Sham) problem is not only well-posed but also Lipschitz stable. We then show that the density-to-potential map is in fact real analytic with respect to both the density and the interaction strength. As a consequence, we obtain a holomorphic extension of the universal constrained-search functional to a suitable subset of complex-valued densities. This partially extends the DFT framework to non-self-adjoint Schrödinger operators. Time permitting, we also discuss two further applications of these results: the existence of an exchange-only part of the exchange-correlation potential, and a rigorous justification of the Görling-Levy perturbation expansion for the correlation energy.

References:

(1) T. C. Corso, "A non-degeneracy theorem for interacting fermions in one dimension" - https://arxiv.org/abs/2503.18440

(2) T. C. Corso , "A rigorous formulation of Density Functional Theory for spinless fermions in one dimension" - https://arxiv.org/abs/2504.05501

(3) T. C. Corso and A. Laestadius, "A quantitative Hohenberg-Kohn theorem and the unexpected regularity of density functional theory in one spatial dimension" - https://arxiv.org/abs/2512.04726

**Constrained Schrödinger Dynamics and the Foundations of TDDFT**

Cancès, Éric (1); Duez, Théo (2); van Gog, Jari (3); Bækgaard Lauritsen, Asbjørn (4); Lewin, Mathieu (4); Toulouse, Julien (3) 17:10

*1: CERMICS, Ecole des Ponts - Institut Polytechnique de Paris and Inria*
*2: CERMICS, Ecole des Ponts - Institut Polytechnique de Paris and Fédération CNRS Bézout*
*3: Laboratoire de Chimie Théorique, Sorbonne Université and CNRS*
*4: CEREMADE, CNRS, Université Paris-Dauphine, PSL Research University*

Density Functional Theory (DFT) has been remarkably successful in describing electronic systems at equilibrium, that is, in the vicinity of their ground states. It has become the reference computational method for large molecules and solids, both in academic research and industrial applications.

By contrast, Time-Dependent Density Functional Theory (TDDFT) remains much less mature and faces significant limitations when addressing fast, strongly out-of-equilibrium phenomena. Developing a sound theoretical foundation for TDDFT, together with reliable approximation strategies, is therefore

a major challenge and would open the way to realistic simulations of a wide range of dynamical phenomena, including charge transfer in complex molecules, electronic response in large systems, and ultrafast phenomena in attosecond physics.

In this work, we revisit the foundations of TDDFT by introducing a general framework for modified Schrödinger dynamics subject to prescribed expectation values of selected observables. The resulting constrained dynamics are rigorously analysed in finite-dimension settings. We show that several natural definitions of constrained Schrödinger dynamics emerge from the underlying geometry of the quantum state manifold. In particular, the conventional formulation of TDDFT can be recovered by imposing stationarity of an action functional, while a purely geometric construction leads to an alternative form of constrained Schrödinger dynamics, which appears to be genuinely different and has not been previously explored.

We conclude by presenting numerical simulations that illustrate the potential of this new approach.

**Fast adaptive discontinuous basis sets for electronic structure**

Pan, Yulong; Lindsey, Michael
*University of California, Berkeley, United States of America*

17:30

We present a discontinuous Galerkin (DG) framework for automatically constructing adaptive basis sets for electronic structure calculations. By allowing basis functions to be discontinuous across element interfaces, our approach supports flexible combinations of atom-centered and polynomial basis sets, maintains favorable numerical conditioning, and induces structured sparsity of the one- and two-electron integrals, which we compute using specialised numerical integration strategies. We also introduce multigrid-preconditioned Poisson solvers that enable fast algorithms for both Hartree-Fock (HF) and density functional theory (DFT) calculations within our DG basis sets. Moreover, these basis sets naturally support adaptive multigrid preconditioning for the linear eigensolvers employed within the self-consistent field iteration for HF and DFT. Numerical experiments for HF and DFT demonstrate that our approach achieves chemical accuracy with modest basis sizes that compare favorably to the sizes of ordinary GTO basis sets achieving similar accuracy, while offering additional structured sparsity and improved computational scalability in the size-extensive limit. The framework thus provides a flexible route toward the construction of systematically improvable and structured adaptive basis sets for electronic structure theory.

**Riemannian Multilevel Optimization for Kohn-Sham Type Problems**

Püschel, Jonas; Vanmaele, Ferdinand
*Universität Augsburg, Germany*

17:50

In this work, we introduce a novel approach to solving Kohn-Sham type problems within the framework of Riemannian multilevel optimization. The Kohn-Sham equations, which are central to density functional theory (DFT) in quantum mechanics, typically present significant computational challenges due to the complexity of electronic structure calculations. To address these challenges, we propose leveraging the geometry of Riemannian manifolds to develop an optimization method that operates over multiple scales or levels of resolution. This multilevel strategy generalizes coarse grid models to the Riemannian framework and enables more efficient convergence by hierarchically refining the solution space, thereby reducing computational costs while maintaining accuracy. We explore the theoretical underpinnings of generic Riemannian multilevel coarse-grid models and illustrate performance in numerical experiments.

**Quantification of Discretization Error in Plane-Wave Density Functional Theory**

Ploumhans, Bruno (1,2); Herbst, Michael (1,2)

*1: Mathematics for Materials Modelling (MatMat), Institute of Mathematics & Institute of Materials, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*
*2: National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland*

18:10

Density functional theory (DFT) is a widely used method in computational chemistry and materials science. It is in principle an exact reformulation of the Schrödinger equation, however practical computations are inexact due to model, discretization, and algorithmic choices. Estimates for these error contributions open opportunities for error balancing, for example by reducing the size of the basis set if other sources of errors are found to be dominating, leading to cheaper simulations with the same overall accuracy.

Plane waves truncated at a so-called kinetic energy cutoff Ecut, are the standard basis set for DFT computations in materials. This talk follows up on promising recent developments by Cancès et al. [1], who proposed an estimate for the discretization error due to the choice of the kinetic energy cutoff. I will briefly review the method and present our strategy to choose its key numerical parameters, with the goal of turning these error estimates into a routinely applicable technique. Finally, I will conclude with a benchmark on an extended set of systems.

[1] E. Cancès, G. Dusson, G. Kemlin, and A. Levitt. "Practical error bounds for properties in plane-wave electronic structure calculations", SIAM Journal on Scientific Computing 44, B1312 (2022).

## S26.06: Excited states calculations

Date: March 19, 2026 08:30–10:30
Room: KI, M11.62
Chair(s): Dusson, Geneviève

**What is your Differential Geometry doing in my Quantum Chemistry?**

Lipparini, Filippo

*Università di Pisa, Italy*

08:30

Many approximated methods in quantum chemistry require one to optimize the molecular energy with respect to various parameters to obtain an optimal wavefunction. Such parameters are usually required to satisfy various constraint, which in textbook quantum chemistry are treated by using Lagrange multipliers or ad-hoc, non-redundant parametrization. An alternative view is that the parameters define a manifold, such as a n-dimensional unit sphere, a Grassmann, or a Flag manifold. In this contribution, I will review a few instances where the geometrical structure of a quantum chemical problem can be exploited to accelerate quantum chemical calculations, focus on two methods: Hartree-Fock or Density Functional Theory in the context of ab-initio molecular dynamics[1-3] and Complete Active Space - Self-consistent Field[4] (CASSCF). In the first example, I will show how the geometric structure of the Grassmann manifold can be exploited to formulate an effective extrapolation strategy that allows us to speed up Born-Oppenheimer molecular dynamics simulations by 20-30% with respect to the state of the art available methods. In the second example, I will detail how Riemannian optimization strategies can be used to optimized the CASSCF wavefunction, a notoriously difficult problem for which finding new optimization strategies is a very active field of investigation. I will the conclude by mentioning other ongoing developments.

[1] Polack et al., *Mol. Phys.* **118,** e1779834 (2020)
[2] Polack et al., *J. Chem. Theory Comput.* **17**, 6965 (2021)
[3] Pes et al., *J. Phys. Chem. Lett.* **14**, 9720 (2023)
[4] Vidal et al., *J. Phys. Chem. A* **128**, 6601 (2024)

**A geometric picture of linear response theory for variational methods**

Grazioli, Laura (1); Hu, Yukuan (1); Nottoli, Tommaso (2); Lipparini, Filippo (2); Cancès, Eric (1) 09:10
*1: Ecole nationale des ponts et chaussées, Institut Polytechnique de Paris and Inria Paris*
*2: Università di Pisa*

In quantum chemistry, the accurate description of excited states is of major interest because of its connection to molecular properties. In the literature, one way to calculate excitation energies as well as molecular properties is linear response theory, which analyses the linearized dynamics around a stable ground state. Although linear response formulations exist for many variational theories, their derivations are often technically involved and rely on ad-hoc constructions. We provide a unified derivation for variational theories by exploiting the geometric structure of Kähler manifolds. The correct parameterization of the manifolds is crucial to correctly define the geometrical tools needed for the construction of a time-dependent dynamics, especially the Riemannian gradient and Hessian. In this work we applied this formalism to the variational theories of Hartree-Fock, described through a Grassmann manifold, and Complete Active Space Self-Consistent Field (CASSCF) theory. We were able to formulate the linear-response equations known in the quantum chemical community as Casida's equations through a simple and universal approach based on Riemannian geometry.

**Making excited state molecular dynamics simulations faster: an extrapolation strategy for linear response TD-DFT**

Nottoli, Michele; Stamm, Benjamin 09:30
*Universität Stuttgart, Germany*

Excited state molecular dynamics (MD) simulations are a powerful computational tool for the study of photo-induced phenomena. A popular method to get the excited state energy and its gradients is linear response time dependent density functional theory (TD-DFT). In this method, the excitation energies and the corresponding perturbations to the electronic density are obtained as eigenvalues and eigenvectors of the molecular response function. The gradients are then used to propagate the classical equations of motion of the molecule.
At each step of an MD simulation, regardless of the method, the new molecular geometry is relatively close to the previous ones. This observation suggests that some extrapolation strategy can be applied, such that the results of the previous calculations (which are available for free) can be used to predict the result of the upcoming calculation. The prediction can then be used as a guess for the iterative solver to lower the number of iterations and thus the cost.
In the case of ground state MD simulations, several strategies extrapolation strategies have been proposed. Among these, the most successful are the extended Lagrangian from Niklasson[1], the GExt scheme from my coworkers[2,3] and Car-Parrinello MD strategies[4]. In the case of linear response TD-DFT MD, only a strategy based on the extended Lagrangian has been proposed so far[5].
In this talk, we first introduce the linear response TD-DFT method for excited states, highlighting its connection with differential geometry. Then, we present an extension of the GExt scheme presented in [3] to linear response TD-DFT, in which the manifold structure to which the solutions belong is used to make the extrapolation more accurate. Lastly, we show how the new extrapolation strategy can be applied to excited state MD simulations, resulting in a significant acceleration.
[1] Niklasson, J. Chem. Phys. 152 (2020).
[2] Polack et al., J. Chem. Theory Comput. 17 (2021).
[3] Pes et al., J. Phys. Chem. Lett. 14 (2023).
[4] Kühne, WIREs Comput. Mol. Sci 4 (2014).
[5] Niklasson et al., J. Chem. Theory Comput. 14 (2018).

**A Constrained Saddle Dynamics for Computing Electronic Excited States**

CANCES, Eric (1); GRAZIOLI, Laura (1); HU, Yukuan (1); LELIEVRE, Tony (1); PARPAS, Panos (2)
*1: CERMICS, École nationale des ponts et chaussées, Institut Polytechnique de Paris and Inria Paris*
*2: Department of Computing, Imperial College London*

09:50

Electronic excited states play a central role in determining the optical and reaction properties of atoms and molecules. Within variational approximate theories, state-specific methods estimate excited states as saddle points of associated energy landscapes defined on Riemannian manifolds. However, these methods often face convergence difficulties due to the intrinsic instability of saddle points, or explicitly involve the computationally expensive Riemannian Hessian. This talk introduces a constrained saddle dynamics on Riemannian manifolds that requires at most (estimates of) Riemannian Hessian-vector products. It couples a position governed by a reflected Riemannian gradient flow with a direction dynamics tracking the lowest invariant subspace of the Riemannian Hessian. By exploiting the underlying Riemannian geometry, we rigorously establish local theoretical results for the dynamics and the resulting discretized algorithm. The effectiveness of the algorithm is examined numerically on standard benchmark systems within restricted Hartree-Fock and complete active space self-consistent field theories.

**Multifidelity Machine Learning for Excitation Energies of Molecular Trajectories**

Vinod, Vivin
*University of Wuppertal, Germany*

10:10

Excitation energies are crucial to understanding essential processes such as photosynthesis. This requires the study of evolution of the excitation energies of a molecule of interest over its trajectory. Performing conventional quantum chemical computations often proves to be a challenge due to the exponential scaling of computational cost associated with the size of the molecule of interest and accuracy, or fidelity, of the method. While machine learning models provide some respite to this they still require a large amount of high fidelity training data to provide reasonable accuracy of prediction. This creates a bottleneck in the pipeline arising from the overhead cost of generating training data.

Multifidelity machine learning aims to address this overhead by utilizing cheaper fidelities in the training of the machine learning models. This talk will introduce the development of novel multifidelity methods with kernel based methods for the prediction of excitation energies along molecular trajectories. Developed methods such as optimized multifidelity machine learning and the Gamma-curve approach will be presented as a low-cost high-accuracy alternative to both conventional quantum chemical computation and single fidelity machine learning methods.

The effectiveness of these methods in reducing the cost of generating training data without sacrificing accuracy will be established for several molecular trajectories ranging from 15 picoseconds simulation of arenes to long simulations of larger and more complex light-harvesting systems such as porphyrins on a clay surface. The talk will conclude with future outlooks and a teasers of simulating an entire light-harvesting complex using multifidelity methods.

## S26.07: Beyond mean-field theories

Date: March 19, 2026 14:00–16:00
Room: KI, M11.62
Chair(s): Hassan, Muhammad

**Recent developments in ab initio tensor network methods**

Legeza, Örs
*Wigner Research Centre for Physics, Hungary*

14:00

We present a brief overview of recent advances in tensor network state (TNS) methods that have the potential to broaden their scope of application radically for strongly correlated molecular systems. We show state-of-the-art results for open shell transition metal clusters obtained via a joint optimization on the matrix product state (MPS) and Grassmann manifolds. We also introduce mixed precision ab

initio TNS methods by utilizing the Ozaki scheme for emulating FP64 arithmetic through the use of fixed-point compute resources. Finally, we showcase recent results obtained on IBM superconducting quantum processor with up to 144 qubits, together with classical validation, using state-of-the-art tensor network simulations via a novel Basis Update Galerkin (BUG) method, establishing agreement between quantum and classical approaches. We close our presentation discussing future possibilities via utilization of Blackwell technology in tree-like TNS calculations opening new research directions in material sciences and beyond.

**Randomised sketching for tensor train rounding: application to quantum chemistry**

Cazeaux, Paul (2); Dupuy, Mi-Song (1); Figueroa, Rodrigo (2) 14:20

*1: Sorbonne Université, Paris, France*
*2: Virginia Tech, Blacksburg, USA*

Randomisation has emerged as a powerful approach in numerical linear algebra, enabling the design of efficient and scalable algorithms for large-scale computations. In this talk, we explore the role of randomisation in the context of tensor trains, a powerful tensor decomposition technique widely used to compute low-lying states in solid-state physics and many-body quantum chemistry. We propose several sketching strategies tailored to improve the tensor-train rounding process, particularly for high-order tensors. The efficiency and accuracy of these randomised methods are illustrated through applications in quantum chemistry.

**The one-body Green's function of quantum lattice systems.**

Kirsch, Alfred 14:40

*Technische Universität München, Germany*

In this talk, I will introduce and discuss the properties of the one-body Green's function, a dynamical reduced quantity in quantum (statistical) physics. After providing a general introduction to the formalism of second quantisation and defining Green's functions, I will demonstrate how certain approximations can be easily formulated within this framework. For example, I will focus on the Hartree–Fock approximation and demonstrate how the Green's function formalism can be used to quantify the error induced by this method.

Furthermore, I will demonstrate how these objects are particularly well-suited to analysing quantum lattice systems, a class of quantum models in which particles are assigned to lie on a discrete (potentially infinite) lattice. These systems are well suited to defining the (generalised) Fourier transform of the Green's function via the thermodynamic limit.

Lastly, the latter quantity can be computed efficiently using Dynamical Mean-Field Theory, an approximate method that has recently come within the scope of mathematical analysis. If time permits, I will introduce this approximation, present existing results, and propose new research directions.

**On a Grassmann manifold optimization problem arising from quantum embedding methods**

NEGRE, Alicia (1); FAULSTICH, Fabian (2); AYRAL, Thomas (3); CANCES, Eric (4) 15:00

*1: CERMICS, Ecole des Ponts - Institut Polytechnique de Paris and Inria Saclay, France*
*2: Department of Mathematics, Rensselaer Polytechnic Institute, Troy, New York, USA*
*3: Department of Quantum Physics, Ecole Polytechnique, Palaiseau, France*
*4: CERMICS, Ecole des Ponts - Institut Polytechnique de Paris and Inria Saclay, France*

Density Matrix Embedding Theory (DMET) is a quantum embedding method designed to study large and strongly correlated quantum systems through a domain-decomposition strategy. In DMET, the central object is the one-particle reduced density matrix (1-RDM) of the global quantum system. The method proceeds by first fragmenting the system into smaller subsystems. These subproblems are then solved iteratively by embedding each subsystem in a bath (the "high-level" stage), while the results are integrated through a self-consistent procedure (the "low-level" stage).

In the conventional DMET formulation, the global 1-RDM is constrained to be a projector. This constraint severely restricts the class of admissible solutions and thus reduces accuracy, particularly in

strongly correlated regimes. The present work investigates how to overcome this limitation by extending the set of admissible 1-RDMs to include mixed states across all key stages of the method. In particular, it proposes an alternative approach for constructing the bath spaces using a Riemannian optimization framework, enabling a more expressive high-level solution. The goal is to enhance the accuracy and flexibility of DMET within a broader framework while remaining consistent with its underlying philosophy. We further relate these developments to recent advances in the field.

**Quantum Algorithm for Real-Space Chemistry: Adaptive Molecular Grids and Transcorrelated Hamiltonian**

Feniou, César (1,2); Cherfan, Christopher (2,3); Zylberman, Julien (1); Claudon, Baptiste (1,2); Piquemal, Jean-Philip (1,2); Giner, Emmanuel (1)
*1: Sorbonne Université, France*
*2: Qubit Pharmaceuticals, France*
*3: Ecole Polytechnique Fédérale de Lausanne, Suisse*

15:20

First-quantized, real-space formulations of quantum chemistry on quantum computers are appealing: qubit count scales logarithmically with spatial resolution, and the two-body Coulomb term achieve quadratic scaling, rather than usual quartic scaling in orbital-based approaches. However, existing schemes employ uniform discretizations whose resolution is imposed by the electron-nuclear cusps of the wave functions in high-density regions, thereby oversampling low-density regions and wasting computational resources. To address this, we repurpose the non-uniform, molecule-adaptive grids long used for DFT integration, which concentrate points where the electronic density is highest, to discretize the molecular Hamiltonian. Once encoded as a quantum operation, its ground state can be obtained with standard Quantum Phase Estimation. We further derive a transcorrelated, non-Hermitian yet isospectral Hamiltonian that removes Coulomb singularities and associated cusps in its eigenfunctions, whose ground-state energy is accessible through the recent generalized Quantum Eigenvalue Estimation protocol. Numerical validation on benchmark systems confirms this ab initio framework paves a promising route to ground-state chemistry on quantum hardware.
This work is closely based on this preprint: https://arxiv.org/abs/2507.20583

**Low-complexity approximations with least-squares formulation of the time-dependent Schrödinger equation**

Dupuy, Mi-Song (3); Ehrlacher, Virginie (1,2); Guillot, Clément (1,2)
*1: École Nationale des Ponts et Chaussées, France*
*2: Inria*
*3: Sorbonne Université*

15:40

We introduce a novel variational formulation for the time-dependent Schrödinger equation, showing that its solution can be uniquely characterized as the minimizer of a global space–time quadratic functional arising from a least-squares principle. The least-squares functional is constructed by reformulating the evolution problem using free dynamics—similarly to scattering theory—and is defined within a space with well-established regularity properties in both space and time. The functional comprises two terms: the first measures the $L^2$ norm of the residual for the twisted evolution equation, while the second enforces the initial condition similarly to a penalty term. We prove that this framework is applicable to the many-body Schrödinger equation with Coulomb singularities by using results from Kato's smoothing theory. Beyond providing a foundation for numerical schemes, this formulation enables the construction of dynamical low-rank approximations based on a variational principle distinct from the classical Dirac–Frenkel approach, and for which global-in-time existence of solutions can be established. In particular, combining the approach with a greedy algorithm, we derive a numerically stable procedure to compute an approximation of the solution as a sum of complex Gaussian wave packets. Since Gaussian wave packets efficiently represent high-dimensional functions with relatively few parameters, the approach remains computationally feasible even in high dimension. While the derivation of a priori bounds for such approximations remains open, our least square functional

naturally yields easily computable a posteriori error bounds. We also investigate the possibility of combining this space-time formulation with an adaptive scheme.

## S26.08: Numerical analysis (Time-dependent problems)

Date: March 19, 2026 17:30–18:30
Room: KI, M11.62
Chair(s): CANCES, Eric

### Regularized dynamical parametric approximation

Feischl, Michael (1); Lasser, Caroline (2); Lubich, Christian (3); Nick, Jörg (4) 17:30
*1: Technische Universität Wien, Austria*
*2: Technische Universität München, Germany*
*3: Univ Tübingen, Germany*
*4: ETH Zürich, Switzerland*

This paper studies the numerical approximation of evolution equations by nonlinear parametrizations with time-dependent parameters , which are to be determined in the computation. The motivation comes from approximations in quantum dynamics by multiple Gaussians and approximations of various dynamical problems by tensor networks and neural networks. In all these cases, the parametrization is typically irregular: the derivative can have arbitrarily small singular values and may have varying rank. We derive approximation results for a regularized approach in the time-continuous case as well as in time-discretized cases. With a suitable choice of the regularization parameter and the time step-size, the approach can be successfully applied in irregular situations, even though it runs counter to the basic principle in numerical analysis to avoid solving ill-posed subproblems when aiming for a stable algorithm. Numerical experiments with sums of Gaussians for approximating quantum dynamics and with neural networks for approximating the flow map of a system of ordinary differential equations illustrate and complement the theoretical results.

### Simulation of the magnetic Ginzburg-Landau equation via vortex tracking

Carvalho Corso, Thiago (1); Kemlin, Gaspard (2); Melcher, Christof (3); Stamm, Benjamin (1) 17:50
*1: IANS-NMH, Stuttgart University*
*2: LAMFA, UPJV and CNRS, UMR 7352*
*3: AA, RWTH Aachen*

In this talk, I will discuss the numerical simulation of the 2D magnetic time-dependent Ginzburg-Landau (TDGL) equations in the regime of small but finite (inverse) Ginzburg-Landau parameter $\varepsilon$and constant (order 1 in $\varepsilon$) applied magnetic field. In this regime, a well-known feature of the TDGL equation is the appearance of quantized vortices with core size of order $\varepsilon$. Moreover, in the singular limit $\varepsilon \to 0$ , these vortices evolve according to an explicit ODE system. After recalling results from the litterature, I will show how to solve in practice this ODE system and how to exploit the trajectories obtained from it to recover an approximate solution to the full TDGL PDE. I will conclude with some numerical simulations, showing that in the dissipative case, we are able to capture the expected criztallization process.

### Numerical Bogoliubov Approximation for Bosonic Quantum Systems

Le Hénaff, Yoann; Lubich, Christian; Pickl, Peter 18:10
*University of Tübingen, Germany*

In this talk we will discuss an algorithm for the numerical simulation of the time-dependent bosonic Schrödinger equation with N particles in the case of a two-body interaction potential, based on the Bogoliubov approximation. This approximation holds in the limit $N \to \infty$, which is what we want to be able to simulate numerically.

By taking naturally into account the symmetries of the system, the Bogoliubov ansatz allows us to obtain a method whose computational complexity is independent of the number of particles. The essential idea consists in representing numerically the condensate function and a small number of

interaction functions that are outside the condensate.
The approximate time evolution of all functions is given by the Dirac-Frenkel time-dependent variational principle. The interaction functions are low-rank approximated and a BUG integrator is used so that the method is robust to small singular values arising from the low-rank approximation. A tensorization property of the interaction functions, given by the Bogoliubov approximation, also allows us to compute the time evolution of only one of them and to deduce the time evolution of all others.

Overall, the numerical scheme we obtain has a computational complexity independent of N.

## S27: Modern teaching and didactics

Organizer(s): Frank, Martin *(KIT)*
Schönbrodt, Sarah *(Salzburg University)*

## S27.01: Modern Teaching: Transition from High-School to University

Date: March 18, 2026 16:30–18:30
Room: KII, M17.24
Chair(s): Frank, Martin

### Supporting transatlantic solution processes for real problems faced by companies: An insight into MINTco@NRW/Authentic-STEM

Stoffels, Gero 16:30
*Universität zu Köln, Germany*

As part of the MINTco@NRW/Authentic-STEM cooperation project between the University of Siegen and the University of Cologne, students aged 14 to 18 are given the opportunity to work on real-life mathematical problems from companies in the fields of production, logistics, commercial, or software development over a longer period of 3-4 months (Stoffels, Schäfer, Köster, & Witzke, 2024). The problems are worked on in internationally mixed solver teams, which meet weekly via a digital collaboration platform to arrive at a joint solution. This presentation will showcase research findings from various fields in the context of the project. The implementation of the project presents several challenges, primarily due to the complexity of the companies' problems and the collaboration structure; the demands placed on the accompanying teachers; and the need to fit the project into regular classroom formats. A particularly high requirement is that the teachers are not experts in the fields of application and, in some cases, have no professional connection to the companies' fields of activity. In addition to investigating critical success factors in the design for integrating such long-term collaborations between schools and companies into regular lessons, the project's stakeholders (students, teachers and company representatives) are also receiving scientific support. With regard to the learners, the research areas include the perception of the problem as involving mathematics (Mathematikhaltigkeit), the application of their skills from mathematics lessons, the self-efficacy experienced during the solving phase of the project, and the natural integration of career-oriented STEM elements. With regard to teachers, our research focuses on teacher competencies, as well as professionalization settings for the expansion of relevant skills. In addition to these developmental research perspectives, concrete use cases and problems from the fields of designing products, big data, and optimization are also presented. The focus here is particularly on the potential of real-world problems to stimulate a variety of mathematical activities and interdisciplinary perspectives. Considering the latter aspect the project contributes to offering meaningful applications of mathematics to students and teachers and to give learners and teachers the opportunity to actively engage with such real-world applications.

Stoffels, G., Schäfer, J., Köster, J., & Witzke, I. (2024). Addressing complexity for educating the future-ready workforce in STEM fields. *LUMAT: International Journal on Math, Science and Technology Education*, *12*(4), 18. https://doi.org/10.31129/LUMAT.12.4.2394

### From Teaching to Learning – Competence Orientation as a Key to Sustainable Learning

Bartel, Thorsten 17:10
*TU Dortmund, Germany*

"Competence orientation" is a central concept in higher education didactics, that is in practice, however, interpreted in very different ways, considered often only superficially, and has so far been implemented only rarely in lectures and courses. Many instructors primarily associate the term with the idea that exam problems should not prescribe a specific solution method but leave the choice of procedure to the students. This widespread reduction to a single aspect is clearly insufficient and does not do justice to the importance of the concept. Instead, competence orientation should be

understood as a counter-model to primarily content-oriented course design. While content-oriented approaches start from specific topics – which are collected, related theories are presented, and, if applicable, suitable exercises are added – competence-oriented conception begins with the intended skills and competences to be achieved by students. Based on clearly formulated learning outcomes, appropriate learning and teaching activities are derived first, followed by assessment formats that make this competence visible in variable situations. Particular emphasis is placed on learning outcomes at higher levels of taxonomy such as analyzing, evaluating, and creating. These outcomes are embedded in the respective disciplinary content, but often target broader and overarching abilities, in particular the critical examination of model assumptions and the results obtained therewith. Once such competences have been achieved, they can be transferred comparatively easily to new problem types and other subject areas. It is precisely this kind of transfer ability that is difficult to achieve with purely content-oriented concepts. The contribution pursues two aims: first, to present a tangible, practice-oriented definition of competence orientation; second, to illustrate with specific examples why competence orientation is a key prerequisite for contemporary university teaching and how this concept can be implemented effectively in higher education practice – in particular in the context of an undergraduate mechanics course.

**From Caesar to RSA: A CAMMP-Based Encryption Workshop for high-school classes**

Heck, Alicia 17:30
*Universität Stuttgart, Germany*

The Computational and Mathematical Modelling Programme (CAMMP, www.cammp.online) offers authentic, competence oriented activities that link mathematics to everyday technology. This paper presents a three hour encryption workshop for students in grade 8 and above, aimed at computer science or mathematics streams.

The workshop pursues three interrelated goals: (i) to raise awareness of the societal relevance of data security, (ii) to introduce the mathematical foundations of modern cryptography—prime numbers, modular arithmetic, and the Euclidean algorithm—and (iii) to provide hands-on experience with both the classical Caesar cipher and public-key RSA encryption using a freely available Jupyter-Notebook environment. Participants start with a brief historical context of secret messages, manually explore Caesar shifts, and then implement RSA key generation and encryption/decryption in the notebook, thereby number-theoretic ideas to concrete digital applications. All instructional materials are released as an Open Educational Resource (OER), enabling easy adaptation across schools and interdisciplinary reuse.

The workshop is built on CAMMP's design principles, exemplified by (a) highlighting the central role of mathematics in cryptographic algorithms, (b) ensuring authenticity and relevance through a real-world data-security scenario, (c) employing the Jupyter-Notebook as an appropriate technical tool, and (d) providing opportunities for discussion, reflection, and internal differentiation within cooperative learning formats. A concise modelling cycle—problem formulation, mathematical modelling, implementation, testing, and evaluation—serves as a metacognitive scaffold throughout the activity.

By integrating these principles, the workshop offers a compact, inquiry-based experience that supports diverse prior knowledge and motivation levels while fostering mathematical competence, ethical awareness, and engagement with technology.

**Development of an Online Course on Numerical Fundamentals**

Born, Tobias; Urban, Karsten 17:50
*Ulm University, Germany*

The „Online course Mathematics In Advanced Studies", or OMIAS for short, is an online mathematics course initiated by the University of Tübingen with the aim of supporting students entering master's programs in the natural sciences. It covers modules on mathematical fundamentals, analysis, linear algebra and ordinary differential equations. The course is available, but development is still ongoing. Access is free of charge and the course is provided in English and German.

This presentation will focus on the development of a new module on numerical fundamentals. It will cover topics in numerical linear algebra (LU decomposition, QR decomposition, computation of eigenvalues, etc.) and numerical analysis (nonlinear systems of equations, polynomial interpolation, numerical integration, etc.).

Online math courses often focus on simpler mathematical topics and limit themselves to describing procedures or providing exercises. Our goal is to teach complex mathematical concepts by combining illustrative derivations, strict mathematical justification, practical exercises and implementation in Python.

We want to take advantage of the benefits that an online course has over traditional lecture materials. Interactive elements let students figure out approaches to problems on their own and encourage them to actively participate. Longer passages of descriptions are broken up by questions and prompts to deduce smaller facts independently. (Interactive) visualizations illustrate content for students and make it visually tangible. Links within the course put topics into context. In general, exercises are randomized, offering the opportunity to practice with changing problem settings. Differentiated feedback on solutions makes it possible to better address students' mistakes. Being able to directly implement learned algorithms in Python and test them on sample problems makes it clear that theoretical derivation and practical implementation are not two separate things, but are inherently linked.

At the same time, mathematical accuracy and completeness are assured. Algorithms are intuitively derived and placed in a mathematical context. Since proofs are essential for understanding numerical approaches, important properties such as the existence and uniqueness of solutions, convergence statements, effort and similar aspects are rigorously proven. The proofs are presented in such a way that students can work them out for themselves under guidance.

**Active Learning – The STEM Exercise Pool for Schools and Universities**

Lohse, Alexander (1); Heimann, Michael (2)
*1: Universität Hamburg, Germany*
*2: integral-learning GmbH, Berlin*

18:10

The STEM Exercise Pool is a digital, interactive teaching and learning resource for mathematics education in the first year of STEM and teacher training degree programs, as well as for upper secondary school. Developed by an team of experts from several universities, it comprises nearly one thousand quality-reviewed tasks featuring automatic grading, differentiated feedback, and dynamic visualizations.

The pool supports a wide range of didactic scenarios, is available in multiple languages, and can be seamlessly integrated into common learning management systems. Technological innovations such as randomized task parameters, LaTeX and Python support, and a web-based authoring tool for collaborative content creation make it a forward-looking instrument for modern, efficient, and motivating STEM education. An integrated AI tutor is currently under development and will further enhance the platform.

## S27.02: Modern Teaching: Modeling & Numerics in Mechanics Education

Date: March 19, 2026 08:30–10:30
Room: KII, M17.24
Chair(s): Bartel, Thorsten

**Sensors in smartphones to support teaching in technical mechanics**

Beitelschmidt, Michael
*TU Dresden, Germany*

08:30

A modern smartphone has a variety of sensors for measuring physical signals. Acceleration sensors in all three spatial directions and angular rate sensors (gyroscopes) for all axes are common. These sensors were originally introduced into the devices to detect haptics. Other built-in sensors may

include a magnetic field sensor and an air pressure sensor. With sampling rates of 200 Hz or more, this enables truly dynamic measurements. The microphone, which is essential for voice communication on the phone, is also a sensor for measuring the physical quantity “sound pressure” with a very high sampling rate. In addition, there is a GPS sensor, which, however, only provides a low sampling rate.

This means that both students and teachers now have a universal dynamics measuring device in their pockets that can be used for demonstrations and self-study. The relevant app-stores offer both free and commercial applications for reading the sensors and processing the corresponding signals, as well as prepared experiments. The following section presents a selection of possible experiments in the fields of dynamics, acoustics, and vibrations.

With the microphone and the appropriate app installed, sound level measurements can be performed. Phenomena such as harmonics and spectrograms can be visualized with a real-time spectrum of the microphone signal.

The built-in acceleration sensors can be used for two types of measurement tasks: With a quasi-static measurement, the speed and distance traveled can be reconstructed from the acceleration signal. This is demonstrated using the example of an elevator ride, in which the air pressure sensor provides valuable additional information. The evaluation of the measurements also reveals possible measurement errors and how they can be corrected.

Dynamic acceleration measurement can be used to detect different modes of oscillating structures. Here too, it is possible to visualize transient vibration processes with the aid of a spectrogram.

The gyroscopes are a particularly useful tool because experience shows that students find it difficult to imagine and understand spatial rotations using body-fixed and inertial coordinate systems. A particularly impressive experiment in this regard is the demonstration of the phenomenon that a rigid body in space rotates stably only around its smallest and largest principal axes of inertia. A smartphone itself is a body that, due to its geometry, has a pronounced spread of its principal moments of inertia. However, it is advisable not to perform the “throwing up with rotation” experiment with the bare phone, but to pack it in a padded body with analog inertial properties. This allows not only the stability and instability of the rotations to be observed, but also measured during flight. The signals from the three rotation rate sensors represent the components of the angular velocity vector in the body-fixed system, as it appears in Euler’s gyroscopic equations. The measurements can be used to confirm the nutation frequency of the stable axes and to observe the transient, unstable movement.

**Gauss’ Principle, Numerical Algorithms and Programming for an Introductory Course on Engineering Dynamics**

Geike, Thomas 08:50
*Berliner Hochschule für Technik, Germany*

Engineering mechanics remains a key element of technical education but continues to pose major challenges for many first- and second-year undergraduate students. In the introductory engineering dynamics class, the author aims for students to be able to establish equations of motion for planar systems of rigid bodies. Students should also be able to solve these equations analytically for simple cases or numerically (usually using the Julia programming language). Additionally, students should have a basic understanding of vibrations with one degree of freedom.

Traditional teaching approaches to elementary dynamics often emphasize analytical derivations based on Newton-Euler and hand calculations, while neglecting opportunities for experimentation, digitalization, and modern computational tools. This paper presents a reorientation through the integration of Gauss’s principle, programming with the Julia programming language supported by generative AI tools (GenAI) and smartphones as measuring devices in the introductory course on engineering dynamics.

Building on previous work that introduced Gauss’s principle of least constraint together with the Python programming language as one cornerstone of elementary engineering dynamics, this contribution demonstrates that the principle can be taught effectively even in first-year courses. Indeed,

using Gauss's principle has many advantages. It well connects to known high school contents (Newton's second law and Gauss's principle of least square), it does not require virtual displacements or velocities, and it allows in many cases to establish the equations of motion without the need to sketch a free-body diagram.

When combined with computational tools, Gauss's principle provides both a conceptual and algorithmic bridge between physical modeling and numerical computation. Using the Julia programming language, students can directly implement the minimization of Gauss's constraint function (using automatic differentiation, numerical minimization or symbolic computation) and explore motion numerically without requiring extensive mathematical expertise for deriving the final form of the equations of motion or solving the equations of motion by hand. That is, modern algorithms such as automatic differentiation or numerical solvers for initial value problems enable students to focus on understanding mechanics rather than on mathematical formalism. Does the use of a programming language in mechanics courses overload students? The author thinks No. GenAI tools are well-known for their effectiveness in supporting programming. They make it easier than ever before to integrate programming into introductory engineering courses.

In conjunction with smartphone-based experiments with the Phyphox App (RWTH Aachen), this integrated approach connects theoretical principles, modern computational mathematics, and tangible experience with practical examples. It thereby contributes both to deep conceptual understanding and to the development of digital competencies essential for future engineers.

**A Practice-Oriented Exercise Concept to Foster Modelling Competence in Technical Mechanics**

Dorschu, Alexandra 09:10
*Hochschule Ruhr West, Germany*

Teaching fundamental concepts of technical mechanics remains a central challenge in engineering education. Students often struggle to transfer theoretical knowledge to real-world problems and to critically reflect on underlying modelling assumptions (Lyon & Magana 2020). Recent research in engineering education emphasizes that active learning approaches—such as problem- or project-based learning—are effective in promoting modelling and problem-solving competences (Sukackė et al. 2022).

To address these challenges, a new exercise concept was developed at the university of applied sciences ,Hochschule Ruhr West, combining hands-on experiences with theoretical strategy training. The first part consists of four practice-based exercises on fundamental topics allowing for inquiry-based and experiential learning. The second part focuses on strategic problem solving, where classical analytical tasks are revisited with explicit emphasis on modelling processes, including simplification, identification of relevant forces, and evaluation of model validity. (Lampe et al. 2023)

The concept was implemented for the first time in the winter term 2025/26. Initial qualitative feedback indicates increased student motivation and a deeper understanding of core mechanics principles. A systematic evaluation using a control-group design is planned for subsequent semesters.

This teaching approach contributes to the ongoing discourse on active learning in engineering education by explicitly connecting practical and reflective phases of learning, the students' ability to link physical phenomena, model formulation, and mathematical representation—key components of modelling competence in engineering.

**Interactive Pluto-notebook to visualize linear-elastic deformations of a tower of a wind turbine based on the Finite Element Analysis**

Cordes, Theresa; Blaszczyk, Mischa; Jänicke, Ralf 09:30
*TU Braunschweig, Germany*

Engineering students often find the Finite Element Method powerful yet abstract. In the early years of study, theoretical concepts are introduced rapidly, leaving little room to see their practical relevance. To address this gap, we have created a Pluto-based FEM notebook that serves as a didactic tool that

invites playful experimentation with various load cases and materials on a “real-world” structure. Our main goal was to develop an interactive, student-friendly tool that makes the mechanical behavior of a simple, but still interesting, structure both visually appealing and easy to explore. As a current relevant example, we selected a wind turbine tower.

We based our analysis on the theory of linear elasticity and implemented the FEM using the Julia package Ferrite.jl [1,2]. The user interface is delivered through a web-based Pluto network [3]. The user can compare the behavior of different pre-meshed tower geometries made of two different materials. It also offers the option to look at various load cases (including wind and gravity). Upon selection, the notebook computes deflections, stress distributions and displacement fields in real time and displays them in 3D-visulizations.

The final tool allows learners to observe how geometry, material, and load interact, and to experiment with different parameters. As a result, this FEM based Pluto-notebook bridges theory and computational practice in solid mechanics and can be used as a lecture accompanying tool.

References:

[1] Kristoffer Carlsson, Fredrik Ekre und Ferrite.jl contributors. Ferrite.jl. url: https: //github.com/Ferrite-FEM/Ferrite.jl.

[2] Jeff Bezanson u.a. „Julia: A fresh approach to numerical computing“. In: SIAM Re view 59.1 (2017), S. 65–98. doi: 10.1137/141000671. url: https://epubs.siam. org/doi/10.1137/141000671

[3] Jeff Bezanson, Stefan Karpinski, Viral B. Shah, and other contributors. Pluto.jl. url: https://github.com/JuliaLang/julia/contributors.

**From Real-World Systems to Physical Models: A Didactic Approach to Fostering Modelling Competence Using the Bicycle in Statics**

Tchomgue Simeu, Arnold; Caylak, Ismail; Ostwald, Richard 09:50
*Paderborn University, Germany*

The gap between abstract theory and its application to real systems poses a significant challenge in engineering studies, particularly in *Engineering Mechanics* 1 (*Statics*), where it often manifests in lower learning outcomes and reduced student motivation. This contribution presents *Bicycle in Statics*, a context-based didactic concept that supports students in identifying system boundaries, making idealizations, and translating real-world systems into physical and mathematical models.

The approach is grounded in *Cognitive Load Theory* and uses the bicycle as a familiar technical reference system to reduce extraneous cognitive load while increasing perceived relevance and motivation. Learning activities follow an iterative four-stage modelling cycle: real-system problem formulation, physical modelling through idealization, mathematical formulation using governing mechanical relations, and verification of results within the original physical context.

The concept is implemented in a digital learning environment within a Moodle-based course using interactive *H5P* modules and *STACK*-based assessments. This setup enables low-threshold activation, immediate feedback, and systematic practice of the bidirectional transition between visual abstraction and analytical formalization. Results from an empirical study, including an expertise comparison between advanced students and instructors, indicate high technical authenticity, increased intrinsic motivation, and strong performance in visual abstraction and mechanical constraint identification. All materials are provided as Open Educational Resources to support reuse and transfer to other teaching contexts.

**Activating Students in Engineering Mechanics: Statics and Strength of Materials in Mechanical Engineering**

Gebhardt, Ulrike; Sähn, Michael; Kästner, Markus 10:10
*TUD Dresden University of Technology, Institute of Solid Mechanics, Germany*

Engineering Mechanics, comprising Statics and Strength of Materials, is a core subject in the foundational curriculum of Mechanical Engineering and is taught over three semesters in the undergraduate program at TUD Dresden University of Technology. Traditionally, the course follows a classical teaching format with lectures for theoretical instruction and exercise sessions in which students solve calculation-based problems independently. While this format ensures systematic coverage of fundamental concepts, it often provides limited opportunities for continuous student engagement and active participation during the semester.

To address this challenge, a set of complementary activation methods has been implemented and is presented and evaluated in this contribution [1]. One method is the integration of a lecture question posed approximately halfway through each lecture. This question takes the form of a practical multiple-choice problem related to the current topic. Students submit their answers via a QR-code-based voting system, after which the results are discussed live in the lecture before continuing with the material. This approach promotes immediate reflection and conceptual discussion. In addition, four lecture quizzes are offered each semester. Each quiz consists of ten multiple-choice questions focusing on conceptual understanding of the lecture content. These quizzes enable students to regularly assess their comprehension and receive timely feedback. Furthermore, the traditional introductory explanation at the beginning of each exercise session has been replaced by short videos that are made available prior to each exercise. Students are encouraged to watch these videos in advance, allowing the in-person exercise time to be used more effectively for independent problem solving and for addressing individual questions. Finally, voluntary learning group assignments are offered in parallel to the regular exercise sessions. Students enroll in semester-long learning groups of up to six participants and collaboratively work on problems whose content has been introduced in the lecture but not yet discussed in the exercises.

Overall, these additional learning activities foster interaction among students as well as between students and instructors. They support continuous self-assessment of learning progress, enable more efficient use of exercise sessions, and provide opportunities to earn bonus points toward the final examination.

[1] Sähn, M., Gebhardt, U., & Kästner, M. (2023). "Mechanics is fun": Course Technical Mechanics - Statics / Strength of Materials - after 2 years of Corona. Lessons Learned, 3(2). https://doi.org/10.25369/ll.v3i2.78

## S27.03: Modern Teaching: AI, Data & Games

Date: March 19, 2026 14:00–16:00
Room: KII, M17.24
Chair(s): Frank, Martin

**Applied Games as Catalysts for Engineering Education**

Freese, Maria 14:00
*Otto von Guericke University Magdeburg, Germany*

"Tell me and I forget, teach me and I may remember, involve me and I learn." This quote from Benjamin Franklin sums up a fundamental truth about learning: true understanding does not come from memorizing formulas or other facts, but from actively experiencing the consequences of one's own decisions, dealing with complexity and uncertainty, and discovering solutions through interactive engagement with others. Accordingly, the question for modern engineering education is: How can learning environments be created that facilitate all of this?

In times characterized by volatility, uncertainty, complexity, and ambiguity, engineering students and professionals inevitably deal with socially relevant topics such as digitalization, sustainability, and the

integration of artificial intelligence. In doing so, they encounter systems with complex cause-and-effect relationships, high dynamics, information density, and conflicting goals that tend to activate intuitive decision-making patterns. This creates an educational necessity to teach not only technical competencies and hard skills, but also future skills such as analytical thinking, complex problem-solving, and critical reflection, which enable future engineers to recognize intuitive reactions and consciously apply sound judgment when complexity requires systematic analysis that goes beyond quick heuristics.

Applied games – whether analogue, hybrid or digital – offer an educational solution by addressing precisely these important future skills in addition to hard skills. Defined as games with a serious purpose beyond entertainment, they prepare future engineers for the challenges and opportunities of digitally connected and dynamic work environments. Applied games act as catalysts in the learning process by creating experimental and safe learning spaces where engineering students can engage with the challenges mentioned above. Unlike traditional teaching formats, these games provide experiential learning environments that encourage active exploration and the acceptance of mistakes as a learning mechanism. They also require systematic reflection. By placing learners in unfamiliar perspectives, applied games promote the development of skills that cannot be adequately taught through theoretical instruction alone. Moreover, they contribute to the understanding of issues that are often perceived as a black box in digitized alternatives.

This presentation will showcase case studies demonstrating how applied games can be understood and utilized as an innovative teaching method in engineering education.

**Teaching in the era of AI**

Kochmann, Dennis M. 14:40
*ETH Zurich, Switzerland*

The capabilities of artificial intelligence (AI) are increasing at an astonishing, if not frightening rate, which has implications on the way we teach and, especially, how our students learn. This is complemented by an every growing offer of online learning tools and course materials. Mechanics and mathematics is no exception. The way we used to teach our classes and educate our students for decades is transforming, which is both a thread and an opportunity. In this (partially philosophical, partially hands-on) talk we will discuss how AI and online tools are shaping and changing our education, including practical examples from AI-based tutors and graders to problem and solution generators. Acknowledging that our students will have to use AI in their professional careers, the aim is not to prevent the use of AI but to teach the responsible use of AI, while also ensuring assessment standards and the promotion of skills and understanding.

**Research-oriented teaching with bwJupyter**

Hoerter, Jasmin 15:00
*Karlsruhe Institute of Technology (KIT), Germany*

Computer-aided modelling and simulations have long been used not only in the natural sciences and technology, but in almost all areas of research, from the social sciences and humanities to medicine. In the rapidly growing field of artificial intelligence in particular, the possible applications are endless. This places new demands on the skills of graduates in all disciplines. To use the numerous tools effectively, training must include not only subject-specific topics but also knowledge of common programming languages and their use in computer-aided calculations. For this to succeed, the entry level should be as low as possible, and the handling should be simple. The open-source software Jupyter satisfies all these requests.

Jupyter notebooks enable interactive and visual representation of research processes, allowing students to engage with scientific methods and data analysis in a practical way. Their use is independent of devices and locations and allows students to easily get in touch with a tool that is well established in research.

By combining code, text and graphics, complex concepts can be communicated in an understandable way and applied directly in real research scenarios. The flexible integration of programming languages such as Python, Julia or R further promotes the development of programming skills.

This presentation will first introduce the functionality of Jupyter Notebooks and then look at the diverse application scenarios and selected case studies. These come from the 'bwJupyter for Teaching' project, a collaboration between KIT and the University of Stuttgart, funded by the Baden-Württemberg Ministry of Science, Research and Arts, which provides a central JupyterHub for all universities in Baden-Württemberg. In its first year of operation, over 7.700 active users from 40 universities were registered.

During the project, various features were developed to support the low-threshold use of Jupyter. Lecturers can create tailor made profiles for their specific courses and include features like a submission function for exercise sheets and a grader service. Moreover, an AI-supported programming assistant was provided to guide newcomers.

The presentation will introduce the use of these and other features in specific teaching scenarios:

1. Classical lecture: Jupyter notebooks are provided as exercise sheets and corrected using the grader service

2. Project work/Hackathon: free, collaborative work by students, use of the programming assistant

3. Thesis: guided work on a specific research project, transition to HPC-cluster

4. Self-study: accessing learning material from the central repository for open educational resources (ZOERR)

**Complex System Modelling with Live Data and Learning - KoSyMo**

Heiland, Jan; Sachs, Sebastian; Cierpka, Christian 15:20
*TU Ilmenau, Germany*

In the age of data and AI, the informed, sustainable and responsible use of data resources is a key competence in the teaching of mathematics and engineering.

In the presented teaching project (in German)

Komplexe Systeme mit Methoden des Maschinellen Lernens modellieren - KoSyMo

we bring together students from engineering and mathematics for an interdisciplinary collaboration on data acquisition, data processing and modelling of a complex physical experiment.

To achieve this, we equip a wind tunnel experiment at the TU Ilmenau with a rather novel but lightweight camera-based measurement device. Thus the setup can be safely operated by students at very low costs and produce a slim data stream that is channelled to the other end of the campus where mathematicians can test their models (and modelling techniques) at real time.

Due to the involvement of live data and models, the differently trained students receive immediate feedback on their efforts and the teams become immediately aware of the challenges and demands of their partner group.

In this talk we want to present the technical setup and discuss first experiences with the experiments and the learnings of the students.

In the near future, reports, implementations, data, and even the interface to the live data will be made available as an open educational resource (OER).

**AR-FLOW: A Unity-Based Platform for Interactive and Structured Learning in Fluid Mechanics**

Aurich, Daniel (1); Sommer-Behr, Alexander (2); Boettcher, Konrad (2); Brümmer, Andreas (1) 15:40
*1: Department of Mechanical Engineering, Chair of Fluidics,TU Dortmund University, Germany*
*2: Department of Biochemical and Chemical Engineering, Laboratory of Equipment Design, TU Dortmund University, Germany*

Teaching fluid mechanics remains challenging due to the abstract and multi-scale nature of many flow phenomena, which are often invisible or difficult to access experimentally. While augmented reality

(AR) and virtual reality (VR) have shown potential to enhance visualization, many existing applications remain isolated demonstrations lacking systematic pedagogical integration.

This contribution presents AR-FLOW, a mobile, Unity-based immersive laboratory platform that has evolved from a visualization tool into a structured, level-oriented learning environment aligned with established educational frameworks. AR-FLOW integrates digital laboratory scripts, interactive AR and VR simulations, and a quest-based learning system grounded in Constructive Alignment and the SOLO taxonomy, guiding students from surface learning toward relational and extended abstract understanding.

Each virtual laboratory is implemented as a modular level focusing on a core fluid mechanics concept, such as the characteristic curves of pumps, 3D flow within a centrifugal pump, potential flow or laminar–turbulent flow transitions. Within each level, students manipulate physical and flow parameters in real time and are guided by structured quests derived from explicitly formulated intended learning outcomes. Immediate feedback and progress tracking support self-directed and self-paced learning.

Technically, AR-FLOW combines real-time interaction with scientifically sound flow visualizations using pre-computed CFD data and analytical solutions, ensuring both performance and conceptual accuracy on mobile devices. The system is designed for scalability and reuse, supporting classroom, laboratory, and home-learning scenarios without the need for specialized hardware or computational resources.

The platform was evaluated in an undergraduate fluid mechanics course using a pre- and post-test design combined with student feedback surveys. The results indicate a moderate overall learning gain above Hattie's hinge point, with medium to large effects for app-specific methodological competencies and students' self-assessed ability to handle real fluid systems, accompanied by a high student acceptance and perceived learning appeal.

By embedding AR and VR visualizations into a coherent instructional design, AR-FLOW bridges the gap between theory and experimentation in fluid mechanics education. The platform demonstrates how immersive technologies can move beyond visualization toward functioning understanding and deep learning, offering a flexible and sustainable approach for modern engineering education.

## S28: Inverse problems, MS2: Dynamics out of equilibrium

Organizer(s): Werner, Frank *(Julius-Maximilians-Universität Würzburg)*
Pietschmann, Jan-Frederik *(Augsburg University)*

## S28.01: Inverse problems

Date: March 17, 2026 08:30–10:30
Room: KII, M17.71
Chair(s): Werner, Frank

### Dimensionality reduction of statistical inverse problems through pretraining

Jahn, Tim 08:30
*TU Berlin, Germany*

We derive error bounds for statistical inverse problems in settings where the effective dimension is reduced by projecting onto subspaces learned from data that only approximately follow the distribution of the true training data. This framework is motivated by recent advances in synthetic pretraining, where subspaces or representations learned from simulated data significantly enhance the feasibility of unsupervised deep learningbased methods such as the Deep Image Prior. These methods have shown remarkable performance in medical imaging inverse problems, despite the scarcity of high-quality real-world training data. Our analysis quantifies the impact of distributional mismatch in the learned subspaces and provides rigorous conditions under which synthetic pretraining yields stable, low-dimensional reconstructions with optimal error guarantees.

### Gamma-convergence of Tikhonov functionals for nonlinear inverse problems

Schuster, Thomas; Hartz, Michael; Belenkin, Alexey 09:10
*Saarland University, Germany*

This talk addresses the problem of $\Gamma$-convergence of a family of Tikhonov functionals and assertions of the convergence of their respective infima. Such questions arise, if model uncertainties, inaccurate forward operators, finite dimensional approximations of the forward solutions and / or data, etc. make the evaluation of the original functional impossible and, thus, its minimizer not computable. But for applications it is of utmost importance that the minimizer of the replacement functional approximates the original minimizer. Under certain additional conditions this is satisfied if the approximated functionals converge to the original functional in the sense of $\Gamma$-convergence. We deduce simple criteria in different topologies which guarantee $\Gamma$-convergence as well as convergence of minimizing sequences. The research presented in the talk is joint work with Alexey Belenkin and Michael Hartz (Saarland University Saarbruecken).

### New Advance Algorithms to Solve Non-Linear Least Square Problem

Farooq, Asma; Guglielmi, Nicola; Tudisco, Francesco 09:30
*Gran Sasso Science Institute, L'Aquila Italy*

Nonlinearity often leads to slow or unstable convergence in iterative solvers for nonlinear least-squares problems. In this work, we introduce a family of accelerated algorithms that leverage a periodically restarted variant of the Generalized Minimum Residual (GMRES) method to address these challenges. The use of restarting strategies not only mitigates computational overhead but also enhances robustness in difficult nonlinear regimes.

To further improve efficiency, our approach integrates sketching and subspace-projection mechanisms, enabling substantial reductions in computational cost while maintaining high solution accuracy. We establish a theoretical framework for the proposed methods, including an explicit perturbation bound that characterizes their stability and sensitivity.

Extensive numerical experiments confirm that the resulting algorithms deliver accurate reconstructions with markedly improved computational performance compared to classical gradient-based techniques.

**The method of the approximate inverse for limited-angle computed tomography**
Schmähl, Richard; Hahn, Bernadette; Rigaud, Gael 09:50
*Universität Suttgart, Germany*

Limited-angle computed tomography stands for one of the most difficult challenges in imaging. Although it opens the way to faster data acquisition in industry and less dangerous scans in medicine, standard approaches, such as the filtered backprojection (FBP) algorithm or the widely used total-variation functional, often produce various artefacts that hinder the diagnosis. With the rise of deep learning, many modern techniques have proven themselves successful in removing such artefacts but at the cost of large datasets. Following a model-driven approach, we propose to take advantage of the method of the approximate inverse. In contrast to FBP-type approaches, our reconstruction technique consists in evaluating linear functionals on the measured data using reconstruction kernels that are precomputed as solution of an auxiliary problem.
This approach avoids the streak artefacts typical for FBP-like reconstructions while recovering all features of the sought-for object. However, it is affected by the severe ill-posedness of the underlying model and requires the design of a tailored regularization strategy, especially when dealing with real measurements. At this aim, we combine spectral filtering, the method of the approximate inverse and custom edge-preserving denoising. In this talk, the proposed approach is mathematically motivated, analyzed and numerically validated for severe limited-angle ranges both on synthetic and real data.

**Learned RESESOP for solving inverse problems with inexact forward operator**
Feinler, Mathias; Hahn, Bernadette 10:10
*University of Stuttgart, Germany*

When solving inverse problems, one often has to deal with potential sources of model inaccuracies, e.g. due to object motion, calibration errors, or simplified data models. Regularized Sequential Subspace Optimization (ReSeSOp) allows to compensate for such inexactnesses within the reconstruction step by employing consecutive projections onto suitably defined subspaces. However, this approach relies on a priori estimates for the model inexactness levels which are typically unknown. In dynamic imaging applications, where inaccuracies arise from the unpredictable dynamics of the object, these estimates are particularly challenging to determine in advance.
To overcome this limitation, we propose a learned version of ReSeSOp which allows to approximate inexactness levels on the fly. The proposed network architecture can be interpreted as a generalization of established unrolled iterative reconstruction schemes, extended to handle inexact forward operators, particularly tailored for dynamic inverse problems. To highlight the strengths of this approach, we analyze the data dependencies inherent in the forward model. This reveals in particular when and why decomposing the overall problem into subproblems is essential. We demonstrate the proposed approach on several dynamic imaging scenarios, including a rheological CT experiment, brain MRI, and real-time cardiac MRI. The results highlight substantial improvements in reconstruction quality while ensuring adequate data consistency.

## S28.02: Inverse problems
Date: March 17, 2026 14:00–16:00
Room: KII, M17.71

**Direct and inverse scattering problems in periodic media**
Zhang, Ruming 14:00
*Technische Universität Berlin, Germany*

Periodic media appear not only in the nature but also play important roles in the modern technologies, such as phototnic crystals, nano-technologies, optical fibers, etc. Driven by its vast applications, mathematicians are also attracted by this topic and have been studying the related topics in the past

decades. In this talk, I will introduce some recent progress in the field of wave propagation problems in periodic media. In particular, I will focus on Helmholtz equations with periodic coefficients or structures. I will present some important and examples for both direct and inverse problems.

**Locally-averaged McCormick relaxations for discretization-regularized inverse problems**

Kaltenbacher, Barbara (1); Manns, Paul (2)
*1: University of Klagenfurt, Austria*
*2: TU Dortmund, Germany*

14:40

As a prototypical coefficient inverse problem, we consider identification of the potential in an elliptic PDE from indirect observations and its regularization by discretization in pre-image space – the so-called least squares version of regularization by projection. We are particularly interested in a situation where the coefficient only takes values in a discrete and finite set. In doing so, we seek to minimize the data misfit over the finite dimensional subspace of piecewise constant function on a given partition of the domain, under the PDE as well as the discrete valuedness as constraints.
The resulting algorithmic challenge is twofold:

* the discretization level must be adapted to the noise level to allow us to stably recover coefficient and state in this nonlinear inverse problem;

* the discretization-regularized minimization problem must be solved to global optimality.

For the former, we establish a general result on the least squares method for nonlinear ill-posed operator equations.
The latter is not possible by gradient-based nonlinear programming algorithms due to non-convexity. We therefore need a global optimization algorithm like (spatial) branch-&-bound, which requires means to compute (approximate) primal upper and dual lower bounds.
In order to obtain dual bounds, we employ a McCormick relaxation, combined with local averaging [1], which reduces the number of degrees of freedom and makes the problem amenable to optimization based bound tightening.
[1] Leyffer, S., Manns, P. McCormick envelopes in mixed-integer PDE-constrained optimization. Math. Program. (2025). https://doi.org/10.1007/s10107-024-02181-1

**On Parameter Identification in Three-Dimensional Elasticity and Discretisation with Physics-Informed Neural Networks**

Caforio, Federica; Holler, Martin; Höfler, Matthias
*University of Graz, Austria*

15:00

Physics-informed neural networks (PINNs) have emerged as a powerful tool in the scientific machine learning community, with applications to both forward and inverse problems. While they have shown considerable empirical success, significant challenges remain—particularly regarding training stability and the lack of rigorous theoretical guarantees, especially when compared to classical mesh-based methods.

In this talk, we focus on the inverse problem of identifying a spatially varying parameter in a constitutive model of three-dimensional elasticity, using measurements of the system's state. This setting is especially relevant for non-invasive diagnosis in cardiac biomechanics, where one must also carefully account for the type of boundary data available.

To address this inverse problem, we adopt an all-at-once optimisation framework, simultaneously estimating the state and parameter through a least-squares loss that encodes both available data and the governing physics. For this formulation, we prove stability estimates ensuring that our approach yields a stable approximation of the underlying ground-truth parameter of the physical system independent of a specific discretisation. We then proceed with a PINN-based discretisation and compare it to traditional mesh-based approaches. Our theoretical findings are complemented by illustrative numerical examples.

**Reducing stability questions for the fractional to the classical Calderón problem**
Baers, Hendrik 15:20
*University of Bonn, Germany*

The Calderón problem is one of the classic examples of an inverse problem. It is about determining the conductivity of a medium by making voltage and current measurements on its boundary. Some of the main questions of interest are about uniqueness and stability of this reconstruction.
In this talk, we will consider the fractional and the classical formulation of the Calderón problem and discuss how these two are related. In particular, we will show that stability estimates for the classical problem can be transferred to stability estimates for the fractional problem.
The results presented in this talk are based on joint work with Angkana Rüland.

**Adjoint-Based Optimization and Parameter Identification for a Volume Penalization Model of Porous Materials**
Schubert, Yannick; Lemke, Mathias 15:40
*TU Berlin, Germany*

In previous work, a volume penalization approach for modeling porous materials in acoustic and aeroacoustic applications was introduced and shown to be suitable for the representation of porous media. The model is formulated within the framework of the compressible Navier–Stokes equations and is characterized by two spatially varying parameters: porosity and length-specific flow resistivity. The spatial dependence of these parameters results in a high-dimensional parameter space, rendering direct optimization and parameter identification computationally challenging.

In the present contribution, an adjoint-based framework is presented for the efficient, gradient-based analysis and identification of the flow resistivity. Starting from the penalized compressible Navier–Stokes equations, the corresponding continuous adjoint system is derived using a Lagrangian formulation. This enables the computation of gradients with respect to the spatially distributed parameters. The inverse problem is formulated through a scalar objective functional defined by the quadratic difference between the simulated solution and a prescribed numerical reference state. As a proof of concept, the methodology is applied to the reconstruction of the macroscopic acoustic and flow-dynamic behavior of a porous-coated cylinder. Validation against numerical reference data demonstrates the accuracy, efficiency, and robustness of the proposed approach. The results highlight the potential of adjoint-based techniques for high-dimensional optimization and inverse problems in acoustics and compressible flow applications involving porous media.

## S28.03: Inverse problems
Date: March 18, 2026 14:00–16:00
Room: KII, M17.71
Chair(s): Pietschmann, Jan-Frederik

**A supervised learning approach for full-field based non-iterative parameter identification**
Brabender, Samuel (1); Rose, Lars (1); Menzel, Andreas (1,2) 14:00
*1: Institute of Mechanics, TU Dortmund*
*2: Division of Solid Mechanics, Lund University*

To solve the inverse problem of material parameter identification, constitutive models are classically calibrated using iterative approaches such as the Finite Element Model Updating method (FEMU). Most modern approaches that introduce Artificial Neural Networks to address inverse problems in this field do not fully exploit their pattern recognition capabilities. Instead, these approaches train Physics-Informed Neural Networks for each new problem, requiring expensive optimisation just as in FEMU.

This work presents a Neural Network-based approach that uses the enhanced pattern recognition capabilities of modern Neural Network architectures. Our method therefor enables direct prediction

of material parameters from full-field displacement and global force data. The network is trained on a comprehensive dataset of simulations, each incorporating unique material parameter sets. Through supervised learning, we establish an effective mapping that enables the Neural Network to accurately predict elastoplastic material parameters for previously unseen datasets. Our approach offers significant advantages for rapid parameter identification, where no further optimisation is required.

**Context-Aware Deep Reinforcement Learning for Adaptive Material Topology Optimization**
Würz, Valentin
*Universität Augsburg, Germany*
14:20

Conventional topology optimization frameworks efficiently minimize structural compliance but rely on homogenized material laws that assume a clear separation of length scales and restrict local material adaptivity. These assumptions often limit achievable performance and fail to account for manufacturability and spatial dependencies efficiently.
To overcome these challenges, we propose a topology optimization framework extended by Deep Reinforcement Learning (DRL) that enables context-aware, element-wise adaptation of material properties under global constraints. The DRL agent performs policy inference on local strain fields to determine optimal material parameters like fiber orientation, volume fraction, and density, which are directly mapped to the element stiffness tensor. This allows the structural response to emerge from full-scale analysis without relying on homogenization assumptions or restrictive parameterizations.
The reward formulation embeds manufacturability and mass constraints, including a discrete set of admissible fiber orientations, penalties for abrupt local transitions, and a global mass budget. Once trained, the agent generalizes across unseen topologies and loading conditions, providing efficient, context-aware material adaptation during inference without the computational burden of repetitive FE2 homogenization.
Building upon earlier work on reinforcement learning for material optimization the proposed framework bridges the gap between topology and material design, extending classical optimization toward manufacturability-aware, context-sensitive, and spatially adaptive structures.

**Generative Design with Uncertainty Based Abstention using Diagonal Flow Matching**
de Campos, Miguel; Gottschalk, Hanno
*TU Berlin, Germany*
14:40

Inverse design describes algorithms which find design parameter specifications $x$ for given performance labels $y_0$. While traditionally forward (surrogate) mappings $y = f(x)$ are used to search for $y^*$, recent generative approaches model a bidirectional invertible mapping $g(y, z) = x$, where $z$ is a latent noise vector such that $x$ and $(y, z)$ are of the same dimension. Sampling of $z$ then provides design alternatives. In this work, we develop a generative inverse design method that is based on a new 'diagonal' conditional flow matching (Diag–CFM) model that is specifically tailored to the inverse design task where it outperforms conditional flow matching (CFM). A problem of flow based generative design is the generation of unreliable solutions, e.g. if the desired labels $y$ are physically infeasible or far outside of the prescribed training set. Here we apply ensemble and gradient based uncertainty quantification to trigger abstention from generation. Our methods are tested on two industrial data sets from airfoil and gas turbine combuster design.

**On an Analytical Inversion Formula for the Modulo Radon Transform**
Beckmann, Matthias
*University of Hamburg, Germany*
15:00

In the recent years, the topic of high dynamic range (HDR) X-ray imaging and tomography has started to gather attention due to advances in hardware technology. The issue is that registering high-intensity projections that exceed the dynamic range of the detector cause sensor saturation, which, in turn, leads to a loss of information. Inspired by the multi-exposure fusion strategy in computational

photography, a common approach is to acquire multiple Radon projections at different exposure levels that are algorithmically fused to facilitate HDR reconstructions.
As opposed to this, in our current line of work, a single-shot approach to HDR tomography has been proposed based on a co-design of hardware and algorithms and modelled the so-called Modulo Radon Transform (MRT), a novel generalization of the conventional Radon transform (RT). In the hardware step, RT projections are folded via a modulo non-linearity, which allows HDR values to be mapped into the dynamic range of the sensor and, thus, avoids saturation. Thereon, recovery is performed by algorithmically inverting the modulo folding so that the MRT measurements are mapped back to the original RT range.
While current MRT reconstruction approaches typically require a low-pass pre-filtering, this talk presents a novel analytical inversion formula for the MRT avoiding bandlimitedness assumptions. It is based on the solution of a Poisson problem linking the Laplacian of the RT of a function to its MRT in combination with the classical filtered back projection formula for inverting the RT. Discretizing the inversion formula using Fourier techniques leads to our novel Laplacian Modulo Unfolding – Filtered Back Projection algorithm, in short LMU-FBP, to recover a function from fully discrete MRT data. Our theoretical findings are finally supported by numerical experiments showing the effectiveness of our approach.
This talk is based on joint work with Carla Dittert (University of Bremen).

**Sparsity-Driven Source Localization for Tomographic Contaminant Sensing**

Mattuschka, Marco (1); An der Lan, Noah (1); Schröder, Stefanie (2); Ficks, Arne (2); von Danwitz, Max (1); Popp, Alexander (1,3)

*1: Institute for the Protection of Terrestrial Infrastructures, German Aerospace Center (DLR), 53757 Sankt Augustin, Germany*
*2: Chemical Detection, Bundeswehr Research Institute for Protective Technologies and CBRN Protection WIS, 29633 Munster, Germany*
*3: Institute for Mathematics and Computer-Based Simulations (IMCS), University of the Bundeswehr Munich, 85577 Neubiberg, Germany*

15:20

Imaging remote sensing systems such as the BRUKER HI90 FPA-FTIR provide high spatial and temporal resolution for detecting airborne contaminants that are invisible to the human eye but potentially hazardous. When two such systems are operated simultaneously and positioned with an appropriate opening angle, they enable tomographic reconstruction of large-scale contaminant plumes with enhanced spatial and temporal accuracy [1].

This contribution presents a modeling framework that leverages these detection capabilities to identify (localize and quantify) the contaminant source. The approach aims to develop a predictive tool for reconstructing release locations based on standoff measurement data, thereby supporting early warning and situational awareness in hazardous release scenarios.

In the proposed method, contaminant transport is modeled using the advection-diffusion equation, and the inverse problem of identifying the unknown source is formulated accordingly. Due to the severe underdetermination inherent to this problem, a sparsity-promoting regularization strategy is employed and the problem is solved using a high-performance optimization algorithm [2]. A corresponding numerical implementation is presented to demonstrate the feasibility of real-time application. Overall, the results illustrate the suitability of the combined sensing and inversion methodology for rapid source localization and plume prediction in operational environments.

[1] Frank Wilsenack, Maria Allers, Fabian Meyer, Thomas Wolf, Torbjorn Tjärnhage, Lars Landström, & Arne Ficks (2024). Combining standoff tomography with point detection: a game changer for the identification of airborne toxic chemicals. In *Chemical, Biological, Radiological, Nuclear, and Explosives (CBRNE) Sensing XXV* (pp. 130560Z). SPIE., https://doi.org/10.1117/12.3013427

[2] Marco Mattuschka, Daniel Walter, Max von Danwitz, & Alexander Popp. (2025). Sparse Source Identification in Transient Advection-Diffusion Problems with a Primal-Dual-Active-Point Strategy, https://doi.org/10.48550/arXiv.2511.02552

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