HAUSDORFF RESEARCH INSTITUTE
FOR MATHEMATICS

UNIVERSITÄT BONN

Workshop

"Taming the PDEs: Tailored Methods, Multiscale Approaches, and Real-World Application"

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organized by
Christian Döding, Andreas Rupp

Abstracts

Gabriel Barrenechea (University of Strathclyde)

Bound-preserving discretisations for general meshes

Abstract: In this talk I will review recent developments a method preserving the bounds of the discrete solution regardless of the geometry of the mesh and the order of the finite element method. The method, recently presented in [1], is built by first defining an algebraic projection onto the convex closed set of finite element functions that satisfy the bounds given by the solution of the PDE. Then, this projection is hardwired into the definition of the method by writing a discrete problem posed for this projected part of the solution. Since this process is done independently of the shape of the basis functions, and no result on the resulting finite element matrix is used, this process guarantees bound-preservation independently of the underlying mesh.
After explaining the main ideas, I will briefly review two recent applications having presenting their own challenges. First, I will discuss the extension to general polytopic meshes [2], where the main challenge lies in the choice of degrees of freedom where the bounds are hardwired. Then, I will move on to the application of this idea to tensor-valued PDEs [3], where a method that preserves the eigenvalue range is presented.

[1] G. R. Barrenechea, E. Georgoulis, T. Pryer, and A. Veeser, A nodally bound-preserving finite element method, *IMA Journal of Numerical Analysis*, 44(4):2198–2219, 2024.

[2] A. Amiri, G. R. Barrenechea, E. Georgoulis, and T. Pryer, A nodally bound-preserving composite discontinuous Galerkin method on polytopic meshes, Preprint, arXiv:2510.02094, 2025.

[3] A. Amiri, G. R. Barrenechea, and T. Pryer, A finite element method preserving the eigenvalue range of symmetric tensors, Preprint, arXiv:2601.04839, 2026.

Lucas Bouck (Carnegie Mellon University)

Commutativity and non-commutativity of limits in the nonlinear bending theory for prestrained microheterogeneous plates

Abstract: In this talk, we discuss the derivation of nonlinear bending models for prestrained elastic plates from three-dimensional non-linear elasticity via homogenization and dimension reduction and numerics for such models. We compare effective models obtained by either simultaneously or consecutively passing to the Γ-limits as the thickness $h << 1$ and the size of the material microstructure $\epsilon << 1$ vanish. In the regime, $\epsilon << h$ we show that the consecutive and simultaneous limits are equivalent, and also analyze the rate of convergence. This talk will also discuss various numerical issues in the computation of the unit cell problem in the regime $\epsilon << h$.

Michael Crocoll (Karlsruhe Institute of Technology)

Scientific Machine Learning for the Ginzburg-Landau equation

Abstract: In this talk, we introduce basic machine learning terminology and techniques. We briefly elaborate on basic network architectures to give a general overview of the machine learning field from our perspective. We then discuss how we used scientific machine learning to approximate minimizers of the Ginzburg-Landau energy. Our approach can be interpreted as learning a parameter-to-solution map. This approximation can be used as an initial guess for suitable iterative solvers or as a standalone method.

Benjamin Dörich (Karlsruhe Institute of Technology)

Approximation of minimizers of the Ginzburg–Landau energy in non-convex domains

Abstract: In this talk, we present our results on discrete minimizers of the Ginzburg–Landau energy in finite element spaces. Special focus is given to the influence of the Ginzburg–Landau parameter. This parameter is of physical interest as large values can trigger the appearance of vortex lattices. Since the vortices have to be resolved on sufficiently fine computational meshes, it is important to translate the size of the parameter into a mesh resolution condition, which can be done through error estimates that are explicit with respect to the Ginzburg–Landau parameter and the spatial mesh width.
In this talk, the main focus is on the influence of non-convex geometries in the approximation process, which in particular effects the magnetic vector potential. Most importantly, we have to choose curl-conforming elements and include the divergence free constraint in a discete manner, and thus deal with a non-conforming method.

Andres Galindo-Olarte (University of Texas at Austin)

A Nodal Discontinuous Galerkin Method with Low-Rank Phase Space Representation for the Multi-Scale BGK Model

Abstract: In this talk, we will present advances in a novel hybrid Discontinuous Galerkin (DG) and Low-Rank approximation method for the BGK equation. This approach aims to reduce computational costs and memory usage while maintaining solution fidelity. It leverages nodal DG discretization for the physical space variables, exploiting the method's flexibility across different geometries, and employs Low-Rank tensors for the velocity space variables. We will also discuss numerical experiments that demonstrate the strengths and limitations of our solver.
This work is a collaboration with Jing-Mei Qiu (University of Delaware), William Taitano (Los Alamos National Laboratory), Mirjeta Pasha (Virginia Tech), and Joseph Nakao (Swarthmore College).

Moritz Hauck (Karlsruhe Institute of Technology)

Guaranteed lower energy bounds for the Gross-Pitaevskii problem

Abstract: We examine the numerical approximation of the ground state of the nonlinear Gross-Pitaevskii eigenvalue problem. Classical conforming discretizations provide upper bounds on the ground state energy because minimization is performed in a subset. In this talk, we present special nonconforming discretization methods that yield guaranteed, asymptotically exact lower energy bounds. We prove the optimal convergence properties of these methods and present numerical experiments that support our theoretical findings.

Patrick Henning (Ruhr University Bochum)

The pollution effect for the Ginzburg-Landau equation

Abstract: The stationary Ginzburg-Landau equation models the appearance of magnetic vortices in superconductors. In this talk we consider regimes where the Ginzburg-Landau material parameter takes large values, as typically the case for high-temperature superconductors. We show the existence of a numerical pollution effect for finite element discretizations of the equation. To be precise, the theoretical resolution condition for meaningful numerical approximations requires the mesh size of the FE space to be smaller than the inverse of the Ginzburg-Landau parameter. However, practically, the smallness condition for the mesh size is much more severe and related to local convexity of the energy. We present corresponding analytical results that quantify the effect and which show that it is reduced in higher order FE spaces, provided that the setting is sufficiently smooth. Furthermore, we illustrate our findings in numerical experiments.

Larissa Martins (National Laboratory for Scientific Computing (LNCC), Brazil)

$H(\mathrm{div};\Omega)$-Conforming Multiscale Hybrid-Mixed Methods for Elasticity with Weak and Strong Symmetry

Abstract: The Multiscale Hybrid-Mixed (MHM) method decomposes the exact solution into global and local contributions. Upon discretization, this leads to a global skeletal formulation coupled with independent Neumann local subproblems, which can be solved using different numerical schemes. In the context of MHM methods for linear elasticity, an attractive strategy for solving the local Neumann subproblems is to employ a Galerkin method using continuous piecewise polynomial spaces for their primal formulation. While computationally efficient, this approach generally yields approximate stress fields that are not $H(\mathrm{div};\Omega)$-conforming, which compromises local conservation and limits the quality of the stress approximation. To overcome this limitation, we introduce and analyze two element-wise reconstruction strategies on submeshes that generate $H(\mathrm{div};\Omega)$-conforming stress tensors while enforcing either weak or strong symmetry of the stress variable. We prove that the reconstructed stress tensor converges optimally in the $H(\mathrm{div};\Omega)$-norm. Moreover, we show that a local projection of the divergence of the approximate stress coincides with the piecewise continuous polynomial projection of the source term onto the submesh, also achieving optimal convergence in the $L^2(\Omega)$-norm with respect to the local mesh size. Numerical experiments confirm the theoretical results and demonstrate the robustness and effectiveness of the proposed strategies in multilayer elasticity problems, aimed at real-world applications such as faulted subsurface reservoirs.

Vishnu Ravenderaan (University of Bonn)

Wave propagation through a time-varying heterogeneous interface

Abstract: We discuss the homogenization and dimension reduction of a wave-type equation with multiple scales in space and time. To perform the homogenization together with dimension reduction we use the method of multi-scale convergence for thin layer which is the generalization of the two-scale convergence for thin heterogenous layer [M. Neuss-Radu, W. Jäger (2007)]. Special attention is given to deriving the transmission condition along the interface. The study should be seen as the preliminary work to design a time-varying metasurface to control wave propagation.

Andreas Rupp (Saarland University)

PDEs in hypergraphs and networks (of surfaces)

Abstract: We introduce a general, analytical framework to express and to approximate partial differential equations (PDEs) numerically on graphs and networks of surfaces – generalized by the term hypergraphs. To this end, we consider PDEs on hypergraphs as singular limits of PDEs in networks of thin domains (such as fault planes, pipes, etc.), and we observe that (mixed) hybrid formulations offer useful tools to formulate such PDEs. Thus, our numerical framework is based on hybrid finite element methods (mainly the class of hybrid discontinuous Galerkin (HDG) methods).
In particular, we notice the beneficial properties of HDG in graphs and consider, as an example, the numerical solution of Timoshenko beam network models, comprised of Timoshenko beam equations on each edge of the network, which are coupled at the nodes of the network using rigid joint conditions. Our discretization of the beam network model achieves arbitrary orders of convergence under mesh refinement without increasing the size of the global system matrix. As a preconditioner for the typically very poorly conditioned global system matrix, we employ a two-level overlapping additive Schwarz method (if the graph is dense).

Katharina Schratz (Sorbonne University)

Resonances as a Computational Tool

Abstract: A large toolbox of numerical schemes for dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever non-smooth phenomena enter the scene such as for problems at low regularity and high oscillations. Classical schemes fail to capture the oscillatory nature of the solution, and this may lead to severe instabilities and loss of convergence. In this talk I present a new class of resonance based schemes. The key idea in the construction of the new schemes is to tackle and deeply embed the underlying nonlinear structure of resonances into the numerical discretization. As in the continuous case, these terms are central to structure preservation and offer the new schemes strong geometric properties at low regularity.

Benjamin Stamm (University of Stuttgart)

Computational methods in Density Functional Theory (DFT)

Abstract: This talk starts with an introduction to the high-dimensional many-body electronic Schrödinger equation and introduces the Kohn–Sham density functional theory (KS-DFT) as a low-dimensional model. We then discuss the mathematical structure of the KS-DFT and present discretization strategies and numerical methods commonly employed in electronic structure calculations. Special attention

is devoted to geometric aspects of the problem, including the representation of electronic states and their intrinsic connection to the Grassmann manifold. Finally, if time-permitting, we briefly outline recent developments in a posteriori error estimation for the total energy in plane-wave KS-DFT to enhance the reliability and efficiency of electronic structure simulations.

Johan Wärnegård (Chalmers University of Technology)

Mathematical modeling of quantum fluids of light

Abstract: In this talk I will introduce the fascinating topic of quantum fluid of lights and the mathematical modeling thereof. Quantum fluids of light have attracted a lot of attention lately due to their ability to achieve strong nonlinear effects and to demonstrate macroscopic quantum phenomena such as superfluidity. In contrast to ultra-cold gases exhibiting superfluidity, these quantum fluids of light constitute open quantum systems as they continually lose photons to the environment and thus need replenishment. This interplay of drive and loss with the fluid-like behavior gives rise to rich and complex physical phenomena, which in turn present both challenges and opportunities to physicists and applied mathematicians alike.

Thomas Wick (Leibniz University Hannover)

A posteriori error control and adaptive discretizations for nonstationary, nonlinear, coupled PDE systems and coupled variational inequality systems

Abstract: In this presentation, we discuss progress over the last decade in adaptive discretizations by different techniques for the accurate, efficient, and robust solution of nonstationary, nonlinear, coupled PDE systems and variational inequality systems (CVIS). First, adaptivity is achieved by goal-oriented error control for single and multiple quantities of interest using the dual-weighted residual method with a partition-of-unity localization. In some projects of our error estimator developments, discretization and nonlinear iteration errors can be balanced. In another recent project, adaptivity is used to select snapshots for a reduced order model with incremental proper orthogonal decomposition. Applications include incompressible flow (Navier-Stokes equations), fluid-structure interaction, phase-field fracture, and model order reduction in porous media. Second, in growing interfaces, such as fractures or damage, adaptivity can also be based on predictor-corrector schemes for the discretization or non-intrusive global-local techniques. Applications include phase-field fracture in porous, thermo-hydro-mechanical propagating fractures, up to thermal-hydraulic-mechanical-chemical fractures. All numerical simulations are substantiated with computational convergence studies and computational cost analyses.

Mahima Yadav (Ruhr University Bochum)

Riemannian optimization methods for computing minimizers of the constrained Gross-Pitaevskii energy in the multicomponent setting

Abstract: This talk considers the Riemannian optimization methods for computing ground states of rotating multicomponent Bose-Einstein condensates, defined as minimizers of the Gross–Pitaevskii energy functional. To resolve the non-uniqueness of ground states induced by phase invariance, we work on a quotient manifold endowed with a general Riemannian metric. We establish a unified local convergence framework for Riemannian gradient descent methods and derive explicit convergence rates. Specializing this framework to two metrics tailored to the energy landscape, we study the

energy-adaptive and Lagrangian-based Riemannian gradient descent methods. While monotone energy decay and global convergence are established only for the former, a quantified local convergence analysis is provided for both methods. Numerical experiments confirm the theoretical results and demonstrate that the Lagrangian-based method, which incorporates second-order information on the energy functional and mass constraints, achieves faster local convergence than the energy-adaptive scheme.
