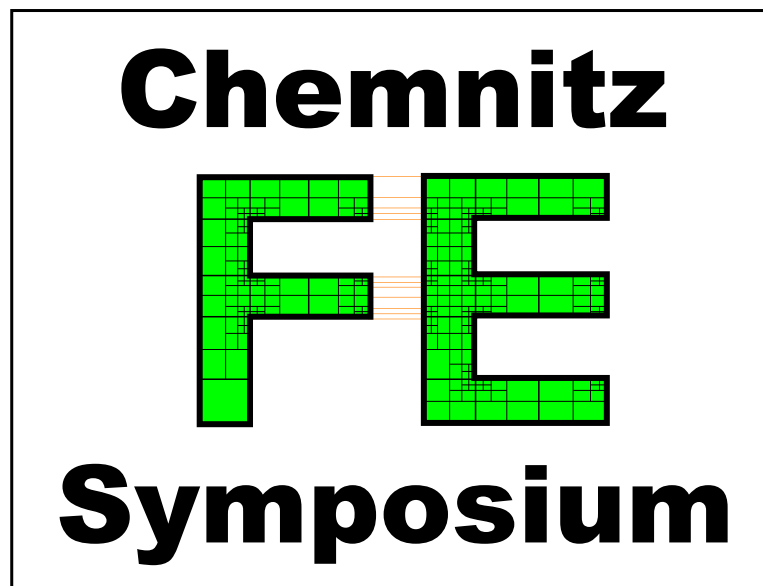

35th Chemnitz FE Symposium 2022

on Tour in Herrsching near Munich



Book of abstracts

Herrsching am Ammersee
September 15 - 17, 2022

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The symposium is devoted to all aspects of computer based solution of partial differential equations.

The topics include (but are not limited to):

- Scientific Computing
- Mechanics/Applications
- Inverse Problems
- Optimization with PDEs
- Uncertainty Quantification

This year we particularly encourage talks on:

- Discretization of problems with low regularity solutions
- Discretization of optimal control problems
- Neural networks with applications to PDEs

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Serge Nicaise (Université Valenciennes)

Joachim Schöberl (TU Wien)

Max Winkler (TU Chemnitz)

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An Adaptive Time Stepping Scheme for Rate-Independent Systems with Non-Convex Energy

Merlin Andreia¹ Christian Meyer²

We investigate a local incremental stationary scheme for the numerical solution of rate-independent systems. Such systems are characterized by a (possibly) non-convex energy and a dissipation potential, which is positively homogeneous of degree one. Due to the non-convexity of the energy, the system does in general not admit a time-continuous solution. In order to resolve these potential discontinuities, the algorithm produces a sequence of state variables and physical time points as functions of a curve parameter. The main novelty of our approach in comparison to existing methods is an adaptive choice of the step size for the update of the curve parameter depending on a prescribed tolerance for the residua in the energy-dissipation balance and in a complementarity relation concerning the so-called local stability condition. It is proven that, for tolerance tending to zero, the piecewise affine approximations generated by the algorithm converge (weakly) to a so-called \mathbb{V} -parametrized balanced viscosity solution. Numerical experiments illustrate the theoretical findings and show that an adaptive choice of the step size indeed pays off as they lead to a significant increase of the step size during sticking and in viscous jumps.

References:

[1] <https://arxiv.org/abs/2204.05860>

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Bioeconomic Model of three marine species in Moroccan Zone with tide effects

Noussaiba Baba¹

The main objective of this work is the study of the effects of high tides and low tides on fishing effort, catches as well as profits in a bioeconomic model of populations of *Sardina pilchardus*, *Engraulis encrasicolus* and *Xiphias gladius* in Moroccan areas. To achieve this objective, we studied the stability of the equilibrium points of our biological model then we added in our model the effect of the tides in the fishing effort which maximizes the profits of the fishermen under the constraint of the conservation of the biodiversity of these marine species using the generalized Nash equilibrium in the resolution of the bioeconomic model. As results, we were able to give the best fishing times according to the tides of each month of the whole year which will allow us to achieve better yields. Hence the importance of introducing the effect of high and low tides in bioeconomic models.

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An intrinsic finite element method for PDEs on surfaces

Elena Bachini¹

Surface PDEs have attracted the interest of many researchers over the last twenty years, due to their applications in various fields from fluid flow to biomedical engineering and electromagnetism. Many proposed numerical approaches rely on an embedding of the surface in a higher-dimensional space. We present here an alternative finite element approach based on a geometrically intrinsic formulation, that we call Intrinsic Surface Finite Element Method (ISFEM). By careful definition of the geometry and the differential operators, we are able to arrive at an approximation that is fully intrinsic to the surface. We consider first a scalar advection-diffusion-reaction equation defined on a surface. In this case, the numerical analysis of the scheme is also available, and we show numerical experiments that support theoretical results. Then, we extend the differential operators for the case of vector-valued PDEs. In this case, the presented formulation allows the direct discretization of objects naturally defined in the tangent space, without the need of any additional projection. Finally, we extend ISFEM to consider moving surfaces via an intrinsic re-definition of the PDE that takes into account a time-dependent metric tensor. To evaluate our approach, we consider several steady and transient problems involving both diffusion and advection-dominated regimes and compare its performance to established finite element techniques.

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Space-time finite element and multigrid methods for coupled hyperbolic-parabolic systems

Markus Bause¹ Mathias Anselmann²

We study the numerical approximation by space-time finite element methods (STFEMs) and the preconditioning of the resulting algebraic problem by geometric multigrid methods for the multi-physics system

$$\rho \partial_t^2 \mathbf{u} - \nabla \cdot (\mathbf{C} \boldsymbol{\varepsilon}(\mathbf{u})) + \alpha \nabla p = \rho \mathbf{f}, \quad (1a)$$

$$c_0 \partial_t p + \alpha \nabla \cdot \partial_t \mathbf{u} - \nabla \cdot (\mathbf{K} \nabla p) = g, \quad (1b)$$

supplemented with initial and boundary conditions. Problem (1) couples hyperbolic elastodynamics with parabolic transport and models poro- and thermoelasticity. Applications of (1) can be found in several branches, including power/reservoir engineering, material sciences and biomechanics/-medicine.

STFEMs allow the natural construction of higher order approximation schemes to (1). They can achieve accurate results on computationally feasible grids. Maintaining the stability and inheriting most of the rich structure of the continuous problem becomes increasingly difficult. Geometric multigrid methods are known as the most efficient iterative methods for the solution of large linear systems arising from the discretization of partial differential equations. To exploit their potential, they need to be adapted to the STFEMs and the mixed hyperbolic- parabolic character of (1).

For its discretization, Eq. (1) is rewritten as a first-order system in time. Galerkin methods in space and time with inf-sup stable pairs of finite elements for the spatial approximation of the unknowns are employed. Optimal order error estimates of energy-type are proven. Superconvergence at the discrete time nodes is addressed further. GMRES iterations with geometric multigrid preconditioning are used for the solution of the algebraic system, involving in parallel all temporal degrees of freedom of the respective subinterval. The performance properties of the parallel V-cycle geometric multigrid preconditioner are investigated carefully by numerical experiments.

References:

[1] M. Bause, U. Köcher, F. A. Radu, Convergence of a continuous Galerkin method for mixed hyperbolic-parabolic systems, IMA J. Numer. Anal., submitted (2022), pp. 1-28; arXiv:2201.12014.

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Eigenvalue problems arising from coupled partial differential equations

Fleurianne Bertrand¹

Determining the response of materials to a given phenomenon is crucial to our description of the world. In particular, recently discovered complex materials with unique features and usually specific microstructure are key to much technology. The corresponding fundamental mathematical problems are eigenvalue problems arising from coupled partial differential equations. In this talk, we discuss spectral properties of operators associated with the corresponding least-squares finite-element minimization of the residual. The convergence of the discrete eigenvalues and eigenfunctions towards the corresponding continuous eigenmodes is studied and analyzed with the help of appropriate L2 error estimates. A priori and a posteriori estimates are proved.

References:

- [1] Bertrand, Fleurianne, and Daniele Boffi. "First order least-squares formulations for eigenvalue problems." *IMA Journal of Numerical Analysis* 42.2 (2022): 1339-1363.
- [2] Bertrand, Fleurianne, and Daniele Boffi. "Least-squares formulations for eigenvalue problems associated with linear elasticity." *Computers & Mathematics with Applications* 95 (2021): 19-27.

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Multilevel adaptivity for stochastic collocation finite element methods

Alex Bespalov¹ David J. Silvester² Feng Xu³

This talk concerns the development of adaptive refinement algorithms for the numerical solution of partial differential equations (PDEs) with uncertain inputs. Sparse grid stochastic collocation representations of parametric uncertainty, in combination with finite element discretization in physical space, have emerged as an efficient alternative to Monte-Carlo strategies, particularly in the context of nonlinear PDE models or linear PDE problems that are nonlinear in the parameterization of the uncertainty.

We present an adaptive algorithm for computing stochastic collocation finite element approximations that employ individually tailored spatial discretizations across collocation points (we call this the multilevel stochastic collocation FEM) [1, 2]. In this algorithm, we employ hierarchical a posteriori estimates for reliable error control in computed approximations and use the associated error indicators to guide the adaptive refinement process; see [1]. The performance of the developed algorithm in numerical experiments for linear elliptic PDEs with non-affine parameterization of uncertain inputs and with parameter-dependent local spatial features will be discussed in detail. In particular, we will demonstrate the effectivity and robustness of the proposed error estimation strategy and discuss the convergence properties of the generated adaptive multilevel approximations.

References:

- [1] <https://arxiv.org/abs/2109.07320>
- [2] <https://arxiv.org/abs/2202.08902>

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Dynamic Pricing in Technology Market

Achraf Bouhmady¹ Nadia Raissi²

A central theme in the marketing of a product is to define a pricing policy that can lead to a market balance. This price dynamic has motivated the development of several mathematical models. The most adapted models to monopol market were introduced by Bass and by Robinson & Lakhani. In this work, we obtain an optimal pricing strategy for the Robinson & Lakhani model by applying necessary optimality conditions. A numerical analysis using Apple's published data, confirms the theoretical result and validates the model.

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- [2] B. Robinson, C. Lakhani, Dynamic Price Models for New-Product Planning. *Management Science* 21, 10 (1975), 1113–1122.
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- [5] R.J. Dolan, A Simulation Analysis of Alternative Pricing Strategies for Dynamic Environments. *Journal of Business*, 1 (1984)

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An hp -Adaptive Finite Element Method for a Chemo-Mechanical Battery Active Particle Model

Fabian Castelli¹ Willy Dörfler²

Lithium-ion batteries are currently the most prominent electrochemical energy storage systems for everyday mobile devices and also large-scale stationary applications. One reason for the decreasing performance of a battery over its lifetime is mechanical stress in the electrode material. An inhomogeneous lithium distribution due to phase separation causes high mechanical stresses, which can induce particle fracture and thus loss of capacity.

We consider our previously developed Cahn–Hilliard-type phase-field model coupling lithium diffusion, large deformations and phase separation based on a thermodynamically consistent transport theory, see [2,3]. Limitations for the numerical investigation are mainly due to the strongly varying spatial and temporal scales of the underlying phase field model, which require a very fine mesh and time resolution, however, solely at specific stages in space and time.

To overcome these numerical difficulties, we present our general-purpose hp -adaptive finite element solution algorithm with variable-step, variable-order time stepping [1].

We show the functionality of the hp -adaptive solution algorithm at the example of the chemo-mechanical particle model and demonstrate the computational savings for an increasing local polynomial degree range. In particular, we compare the developed method to one with fixed spatial degree and observe reduction of the computational cost.

References:

- [1] G.F. Castelli, W. Dörfler: Comparison of a h - and hp -adaptive finite element solver for chemo-mechanically coupled battery electrode particles. Submitted. 2021.
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p-Adaptive discontinuous Galerkin method for Richards' equation solution

Jean-Baptiste Clément¹

Flows in variably-saturated porous media are described by Richards' equation whose numerical solving can be troublesome and costly because of abrupt changes in the nonlinear hydraulic properties [1]. Typically, Richards' equation exhibits sharp wetting fronts moving dynamically in the unsaturated zone while the saturated zone remains relatively smooth. In that context, local adaptation of mesh discretization (h-adaptation) or space order approximation (p-adaptation) can improve the computational efficiency. This work aims to investigate p-adaptation which is known to reach accuracy with a reduced cost compared to low-order methods [2]. To this end, Richards' equation is solved by discontinuous Galerkin methods [3] whose properties make them appealing for locally adaptive high- order approximation. In this study, the p-adaptative algorithm is kept simple in order to make extension to hp-adaptation as easy as possible in the future. Benefits for Richards' equation are evaluated. Results from numerical experiments demonstrate the potential of p-adaptation for Richards' equation.

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- [3] V. Dolejší and M. Feistauer. *Discontinuous Galerkin Method*. Springer International Publishing, (2015).

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Space-Time Finite Elements and Model Order Reduction

Max von Danwitz¹ Fabian Key² Norbert Hosters³ Marek Behr⁴

Space-time finite element methods provide a combined discretization of space and time for the numerical solution of partial differential equations (PDEs). In this contribution, we study space-time discretizations for time-dependent scalar transport and flow problems.

As a prototype test, the convergence behavior of time-discontinuous space-time finite element methods is numerically investigated for a scalar advection-diffusion model problem. Therein, the model parameter choices include the parabolic and hyperbolic limit cases. The computational error analysis demonstrates temporal superconvergence of prismatic space-time finite elements for parabolic problems [1].

After tests of the prototype, this contribution focuses on heat flux and fluid flow applications with simplex space-time meshes [2]. For such applications, there is a large demand for solutions that are fast to evaluate with limited computational power, yet, lay within reasonable accuracy bounds. E.g., in the context of digital twins, fast-to-evaluate models are required to interact with sensor data of the real system under consideration. To address this issue, a reduced-order model (ROM) can be obtained through the application of a projection-based Model Order Reduction (MOR) approach [3]. We report first results of a MOR approach for deforming domain problems based on space-time finite elements.

References:

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- [2] <https://onlinelibrary.wiley.com/doi/epdf/10.1002/fld.4743>
- [3] <https://onlinelibrary.wiley.com/doi/epdf/10.1002/pamm.202100071>

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The Magnetic Polarizability Tensor for the Classification and Characterisation of Different Metallic Objects

James Elgy¹ Paul Ledger²

Low frequency metal detection is important for applications including terrorist object identification, such as knives and firearms; scrap metal sorting, archaeological surveys, and the identification of unexploded ordnance. However, current metal detectors are not able to distinguish between different shapes, small objects buried at shallow depths, and larger objects buried at greater depths. It is known that a hidden conducting object can be characterised by a complex symmetric rank 2 Magnetic Polarizability Tensor (MPT), which is a function of the object's size, shape, conductivity, permeability, and the frequency of excitation. The MPT provides an ideal object characterisation, which can be combined with a machine learning classifier. We present ongoing work concerning using finite element simulations for the classification and characterisation of small metallic objects when testing with measured MPT signatures, their validity, and the challenges associated with introducing high permeability objects.

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- [2] Wilson, B. A., Ledger, P. D., & Lionheart, W. R. B. (2022). Identification of metallic objects using spectral magnetic polarizability tensor signatures: object classification. *International Journal for Numerical Methods in Engineering*, 123(9), 2076–2111.

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Weighted analytic regularity and hp-FEM for the integral fractional Laplacian

Markus Faustmann¹ Carlo Marcati² Jens Markus Melenk³ Christoph Schwab⁴

In this talk, we consider PDEs involving fractional powers of the Laplacian $(-\Delta)^s$ for $s \in (0, 1)$, using the singular integral definition. Solutions to fractional PDEs are known to lose regularity near the whole boundary of the computational domain.

On polygonal domains, we establish a precise description of the regularity of solutions for analytic data in suitably weighted Sobolev spaces reflecting both the analytic nature inside the domain and the anisotropic singular behaviour near the boundary. Unlike local elliptic operators in polygons, fractional operators in polygons require not only vertex-weighted but also additionally edge-weighted spaces.

Weighted analytic regularity results of our type can be used to design exponentially convergent hp -finite element approximations on suitable anisotropic geometric meshes.

References:

[1] M. Faustmann, C. Marcati, J.M. Melenk, Ch. Schwab *Weighted analytic regularity for the integral fractional Laplacian in polygons*, arXiv:2112.08151 (2021)

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Implicit Runge-Kutta schemes for optimal control problems with evolution equations

Thomas Flaig¹

In this presentation we discuss the use of implicit Runge-Kutta schemes for the time discretization of optimal control problems with evolution equations. The specialty of the considered discretizations is that the discretizations schemes for the state and adjoint state are chosen such that discretization and optimization commute. It is well known that for Runge-Kutta schemes with this property additional order conditions are necessary. We give sufficient conditions for which class of schemes these additional order condition are automatically fulfilled. The focus is especially on implicit Runge-Kutta schemes of Gauss, Radau IA, Radau IIA, Lobatto IIIA, Lobatto IIIB and Lobatto IIIC collocation type up to order six. Furthermore we also use a SDIRK (singly diagonally implicit Runge-Kutta) method to demonstrate, that for general implicit Runge-Kutta methods the additional order conditions are not automatically fulfilled.

Numerical examples illustrate the predicted convergence rates.

The talk is based on the preprint [1].

References:

[1] <https://arxiv.org/abs/1311.0640>

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Numerical simulations of first order systems

Sebastian Franz¹

In this talk we consider problems of the class

$$(\partial_t M_0 + M_1 + A)U = F,$$

where ∂_t stands for the derivative with respect to time, $M_0 : H \rightarrow H$ and $M_1 : H \rightarrow H$ are bounded linear selfadjoint operators on some Hilbert space H , $A : D(A) \subset H \rightarrow H$ is an unbounded skew-selfadjoint operator on H and F is a given source term.

Many if not all physical linear problems fall into this class, including but not limited to convection-reaction-diffusion problems, linear elasticity and Maxwell's equations. We are interested in numerical methods for above problems and present some recent results including a singularly perturbed problem and homogenisation of Maxwell-type problems.

References:

- [1] <https://doi.org/10.1093/imanum/dry007>
- [2] <https://doi.org/10.1007/s10915-021-01638-1>
- [3] <https://doi.org/10.1002/mma.1110>

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Mixed Finite Element Method for 2nd Order Dirichlet Boundary Control Problem

Divay Garg¹

The optimal control problems (OCPs) subjected to partial differential equations (PDEs) have numerous applications in fluid dynamics, image processing, mathematical finance etc. The objective of OCPs is to find the optimal control which minimizes/maximizes the given cost functional with certain constraints (mainly in form of PDEs) being satisfied. There are mainly two types of OCPs available in literature namely, Distributed Control Problems where the control acts on the system through an external force and Boundary Control Problems where the control acts on the system through a Dirichlet or Neumann or Robin boundary conditions. Dirichlet boundary control problems are difficult to handle due to variational difficulty.

In many applications, it is important to obtain accurate approximation of the scalar variable and its gradient simultaneously. A common way to achieve this goal is to use mixed finite element methods. The main aim of my talk is to analyze the mixed finite element method for the second order Dirichlet boundary control problem in which the control is penalized in the energy space. Mixed finite element methods have the property that they maintain the discrete conservation law at the element level. For the variational formulation, the state equation is converted to the mixed system using the mixed variational scheme for second order elliptic equations and then the continuous optimality system is derived. In order to discretize the continuous optimality system, the lowest order Raviart-Thomas space is used to numerically approximate the state and costate variables whereas the continuous piece-wise linear finite element space is used for the discretization of control. Based on this formulation, the optimal order a priori error estimates for the control in the energy norm and L_2 -norm is derived. The reliability and the efficiency of proposed a posteriori error estimator is also discussed using the Helmholtz decomposition. Finally, several numerical experiments are presented to confirm the theoretical findings.

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- [3] F. Trolzsch. *Optimale Steuerung Partieller Differentialgleichungen*. Viweg, Cambridge University Press, 2005.

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On shape optimization with parabolic state equation

Helmut Harbrecht¹ Rahel Brügger² Johannes Tausch³

This talk is concerned with the solution of time-dependent shape optimization problems. Specifically, we consider the heat equation in a domain which might change over time. We compute Hadamard's shape gradient in case of both, domain integrals and boundary integrals. As particular examples, we consider the one-phase Stefan problem and the detection of a time-dependent inclusion. Numerical results are given.

References:

[1] <https://doi.org/10.1137/21M1411007>

[2] <https://doi.org/10.1137/19M1268628>

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Optimal control and regularization of a simplified Signorini problem

Christof Haubner¹

In the context of optimal control we consider a simplified Signorini problem, an elliptic variational inequality of first kind with unilateral constraints on the boundary. The state is discretized using linear finite elements while a variational discretization is applied to the control. We derive a priori error estimates for control and state based on strong stationarity and a quadratic growth condition. The convergence rates depend on H^1 and L^2 error estimates of the simplified Signorini problem.

We verify the theoretical findings with numerical tests, which are done by considering a regularized problem. The corresponding regularization error is also discussed.

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An Optimal Time Variable Learning Framework for Deep Neural Networks

Evelyn Herberg¹ Harbir Antil² Hugo Diaz³

Feature propagation in Deep Neural Networks (DNNs) can be associated to nonlinear discrete dynamical systems. The novelty, in this paper, lies in letting the discretization parameter (time step-size) vary from layer to layer, which needs to be learned, in an optimization framework. The proposed framework can be applied to any of the existing networks such as ResNet, DenseNet or Fractional-DNN. This framework is shown to help overcome the vanishing and exploding gradient issues. Stability of some of the existing continuous DNNs such as Fractional-DNN is also studied. The proposed approach is applied to an ill-posed 3D-Maxwell's equation.

References:

[1] <https://arxiv.org/abs/2204.08528>

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Efficient Solution of A Nonlocal Optimal Control Problem

Roland Herzog¹

We consider the optimal control of a Kirchhoff-type problem, which is governed by a partial differential equation with a nonlocal term. Consequently, the linear systems arising in the solution of the forward problem and also the optimality system associated with an optimal control problem, contain dense blocks. We discuss a preconditioning strategy for iterative solvers and a matrix-free implementation, which significantly cuts down on the computational cost. Analysis and numerical results are presented.

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PDE constrained shape optimization in the Lipschitz topology

Michael Hinze¹ Klaus Deckelnick² Philip Herbert³

We propose to perform PDE constrained shape optimization using the method of mappings with descent realized in the Lipschitz topology. We present numerical analysis, and also conduct numerical examples which indicate that minimization in the Lipschitz topology seems to be superior over the classical minimization in Hilbert spaces, in particular when the optimal shape has sharp corners. Moreover, on the implementation level, mesh degeneration during the minimization procedure is avoided with our approach.

References:

[1] <https://www.esaim-cocv.org/articles/cocv/abs/2022/01/cocv210048/cocv210048.html>

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Finite element methods respecting the discrete maximum principle for convection-diffusion equations I

Volker John¹ Gabriel R. Barrenechea² Petr Knobloch³

Convection-diffusion-reaction equations model the conservation of scalar quantities. From the analytic point of view, solution of these equations satisfy under certain conditions maximum principles, which represent physical bounds of the solution. That the same bounds are respected by numerical approximations of the solution is often of utmost importance in practice. The mathematical formulation of this property, which contributes to the physical consistency of a method, is called Discrete Maximum Principle (DMP). In many applications, convection dominates diffusion by several orders of magnitude. It is well known that standard discretizations typically do not satisfy the DMP in this convection-dominated regime. In fact, in this case, it turns out to be a challenging problem to construct discretizations that, on the one hand, respect the DMP and, on the other hand, compute accurate solutions.

This talk starts to presents a survey on finite element methods, with a main focus on the convection-dominated regime, that satisfy a local or a global DMP. The concepts of the underlying numerical analysis are explained. Some linear discretizations with P_1 finite elements satisfying DMPs are described. Linear discretizations for other finite elements are discussed briefly.

Part II of this talk will be presented by Petr Knobloch. This topic is joint work with Gabriel R. Barrenechea and Petr Knobloch.

References:

[1] <https://arxiv.org/abs/2204.07480>

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Anisotropic and pressure-robust discretization of incompressible flows

Volker Kempf¹

For some time, the class of pressure-robust discretizations for incompressible flows has sparked increased interest. They produce velocity approximations that are independent of how well the pressure can be approximated, and are highly advantageous in low viscosity regimes. While classical methods like the family of Taylor–Hood finite elements show a locking phenomenon induced by the viscosity parameter of the fluid, meaning that the error of the discrete velocity solution scales with the inverse of the viscosity, pressure-robust methods do not have this problem.

Incompressible flows tend to form layer structures, e.g., near walls, and exhibit singular solutions near re-entrant edges of the domain. These two effects cause additional difficulties for discretization approaches that can be addressed by anisotropic mesh grading, which uses highly stretched elements in boundary layer regions or near the re-entrant edges. A drawback with regard to the use of anisotropic grading is that proofs are available for only a few methods.

The talk focuses on the pressure-robust variants of the Crouzeix–Raviart and Bernardi–Raugel methods and their performance in the context of anisotropic meshes. Numerical examples are presented that support the results from the analysis.

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Finite element methods respecting the discrete maximum principle for convection-diffusion equations II

Petr Knobloch¹ Gabriel R. Barrenechea² Volker John³

This talk is a second part of a joint presentation with Volker John (see the abstract of Part I for an introduction into the topic). The talk will be devoted to the numerical solution of both steady-state and time-dependent convection-diffusion-reaction equations and, in contrast to Part I, it will present examples of nonlinear finite element methods satisfying the discrete maximum principle (DMP). In fact, it turns out that, for steady-state problems, all successful finite element approaches satisfying the DMP are nonlinear, which will be also illustrated by numerical results. The talk will concentrate on conforming P_1 finite elements and results for other types of finite elements will be mentioned only briefly.

This talk is based on a joint review paper with Gabriel R. Barrenechea and Volker John.

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Application of fully implicit Nested Newton solvers to multicomponent multiphase flow in porous media and to elastoplastic deformations of biological tissue

Markus M. Knodel¹

Advanced models of complicated physical and biological processes incorporate huge equation systems which combine partial differential equations (PDEs), ordinary differential equations (ODEs), and algebraic equations (AEs).

The monolithic solution of such extended equation systems all together using standard techniques sometimes is very time consuming due to the highly nonlinear couplings linking the PDEs, ODEs, and AEs. The application of operator splitting methods as well often is highly time consuming, as very small time steps often are needed in such cases.

The application of nested Newton solvers allows to shift a substantial part of the nonlinear computations to the so-called local system containing only non-spatially coupling equations (ODEs, AEs). The global equations contain all PDEs and are hence spatially connected. If the local variables are coupled with the global variables by means of a so-called resolution function, the solution technique remains monolithic and fully implicit. The number of the local Newton steps (which can be performed with perfectly parallel scalability) displays an upper bound for the global Newton steps, which contain the spatial couplings.

We present two examples of applications of a nested Newton algorithms which allow the efficient evaluation of the corresponding models:

In order to study the efficiency of the various forms of trapping including mineral trapping scenarios for CO₂ storage behaviour in deep layers of porous media, we apply the globally fully implicit PDE reduction method developed 2007 by Kräutle and Knabner for one-phase flow extending the method to the case of an arbitrary number of gases in gaseous phase. The advective parts of the Finite Element discretized PDEs are stabilized with cell centered Finite Volumes. We present scenarios of the injection of a mixture of various gases into deep layers, we investigate phase change effects in the context of various gases, and study the mineral trapping effects of the storage technique.

Further, we simulate elastoplastic deformation of biological tissue with anisotropic structure in case of a highly nonlinear material model developed by Di Stefano and Grillo. Applying the BilbyKrönerLee (BKL) multiplicative decomposition of the deformation gradient into an elastic and a plastic part, a natural split into local and global system is achieved. The PDEs representing the virtual powers are discretized by means of Finite Elements. We compare the simulations for the case of isotropic and anisotropic material and find substantial differences in the properties of the material stress response depending on the velocity of the material deformation.

Our applications demonstrate the potential of nested Newton procedures for efficient solution techniques in case of highly nonlinear models of complicated scenarios.

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Globalization of Nonlinear FETI-DP Methods

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Nonlinear FETI-DP (Finite Element Tearing and Interconnecting – Dual-Primal) methods are domain decomposition methods for the solution of nonlinear problems from the discretization of PDEs. In these methods, before linearization, the global problem is decomposed into concurrent nonlinear problems. Then, different local elimination strategies can be used, in the sense of nonlinear preconditioning. This talk discusses (exact) penalty methods for the globalization of Nonlinear FETI-DP methods.

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Modeling of two-phase flow in porous media: transport behavior of lubricant oil in rubberwood

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Nowadays, eco-friendly technologies for separation of oil/water mixtures have been developed. Wood becomes a promising material for a conduit for fluid flow due to its natural hierarchical structure and high porosity. However, due to the structural complexity of the wood, the oil transport in wood is difficult to be monitored. Synchrotron X-ray Tomographic Microscopy (SR-XTM) is a reliable and robust technique to observe the oil transport in real geometries of wood. This work presents monitoring of the lubricant oil transport behavior in rubberwood using the SR-XTM. Additionally, a numerical model solved using a finite element analysis (FEA) with phase field method and creeping flow model is conducted on the lubricant oil transport in rubberwood to predict the time-dependent fraction of lubricant oil within rubberwood. The model results are compared with experimental data. The lubricant oil transport in rubberwood demonstrates that the lubricant oil advances along the efficient transport pathways which are vessel cells. However, the closed vessel cells act as a barrier of oil transport that would affect a reduction of oil flux. It is also found that the surface tension has a great effect on the liquid flowing through the microstructure of rubberwood. The SR-XTM technique combined with the simulation obtained from this work opens new horizons for exploring a wide range of permeable materials for oil separation and also extends the wide applications of wood.

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The Impact of Artificial Intelligence on Partial Differential Equations: From Successes to Limitations

Gitta Kutyniok¹

Artificial intelligence is currently leading to one breakthrough after the other, both in public life with, for instance, autonomous driving and speech recognition, and in the sciences in areas such as medical diagnostics or molecular dynamics. A similarly strong impact can currently be witnessed on scientific computing such as for solvers of partial differential equations.

In this lecture, we will first provide an introduction into this new vibrant research area. We will then specifically focus on high-dimensional parametric partial differential equations (PDEs), which appear in various contexts including control and optimization problems, inverse problems, risk assessment, and uncertainty quantification. Recently, numerical experiments demonstrated the remarkable efficiency of using deep neural networks to solve parametric problems. In the second part of this talk, we will provide a theoretical justification for this class of approaches in term of approximation-theoretical results. Moreover, we will present a comprehensive numerical study of the effect of such results for neural networks on practical learning problems. We will finish with a word of caution when training neural networks for solving PDEs on classical digital hardware, and present fundamental limitations.

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Pointwise error estimates for C^0 interior penalty approximation of biharmonic problems

Dmitriy Leykekhman¹

In this talk we will discuss pointwise error estimates for the biharmonic equation on a convex polygonal domain. Finite element discretization of this problem is not straightforward and various approaches were proposed over the years. However, they all have some drawbacks. The C^0 interior penalty method is a sound alternative. This method is attractive since the finite elements consist of usual Lagrange elements of arbitrary order and it is straightforward to implement. Pointwise error estimates is a well-developed area for the second order problems, however, there are few such results for fourth order problems. Many such pointwise error estimates are obtained via Sobolev embedding. This is not satisfactory since such results are usually not optimal and often the discrepancy between norms makes them hard to use for applications, for example, for optimal control problems. In addition, it is hard to localize them. I will discuss an approach based on dyadic domain decompositions and local energy estimates that allow us to obtain the best approximation global and local type results for the second derivative. In this talk we will discuss the main ideas of the proof and highlight the major differences between the analysis of the second and fourth order problems.

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Adaptive FEM for distributed optimal control problems subject to the wave equation with variable energy regularization

Richard Löscher¹ Olaf Steinbach²

We present a space-time finite element approach for a distributed optimal control problem for the wave equation. We will consider the cases of $L^2(Q)$ - and energy regularization, using a modified variational formulation and a suitable solution space for the wave equation for the latter. A comparison between both approaches, in particular in view of the optimal choice of the relaxation parameter, is carried out. Numerical examples, including an adaptive refinement strategy, are given.

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Finite Element Method for the Generalized Burgers-Huxley Equation with Memory

Sumit Mahajan¹ Arbaz Khan² Manil T. Mohan³

In this talk, we will address the analysis and the numerical approximation of the 2, 3-dimensional generalized Burgers-Huxley equation with memory (a non-linear advection-diffusion-reaction problem). Firstly, the existence of a unique solution to the continuous problem have been obtained using the Faedo-Galerkin approximation method. Under smoothness assumptions on the initial data and the external forcing, we will derive further regularity results of the weak solution. Secondly, for the numerical studies, we propose a conforming finite element method for its numerical approximation using backward Euler discretization in time. Further, A prior error estimate for the approximation is also derived. Finally, the computational results are presented to support the derived theoretical results.

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Operator compression with deep neural networks

Roland Maier¹ Fabian Kröpfl² Daniel Peterseim³

We study the compression of partial differential operators using neural networks. We consider a family of operators, parameterized by a potentially high-dimensional space of coefficients that may vary on a large range of scales. Based on the existing methods that compress such a multi-scale operator to a finite-dimensional sparse surrogate model on a given target scale, we propose to directly approximate the coefficient-to-surrogate map with a neural network. We emulate local assembly structures of the surrogates and thus only require a moderately sized network that can be trained efficiently in an offline phase. This enables large compression ratios and the on-line computation of a surrogate based on simple forward passes through the network is substantially accelerated compared to classical numerical upscaling approaches. We apply the abstract framework to a family of prototypical second-order elliptic heterogeneous diffusion operators as a demonstrating example.

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The neural network multigrid solver for the Navier-Stokes equations and its application to 3D simulation

Nils Margenberg¹ Robert Jendersie² Dirk Hartmann³ Christian Lessig⁴ Thomas Richter⁵

Our work extends the Deep Neural Network Multigrid Solver (DNN-MG) introduced in [1] by an online learning approach and the application to 3D flow simulation. DNN-MG is a novel method for machine learning enhanced simulations, which improves computational efficiency by a combination of a geometric multigrid solver and a recurrent neural network. The multigrid solver is used in DNN-MG for the coarse levels while the neural network corrects interpolated solutions on fine levels, avoiding the increasingly expensive computations. DNN-MG uses the neural network to correct local patches of the mesh domain. This greatly facilitates generalizability and allows us to use a network trained on one mesh domain also on a different one. The locality also results in a compact neural network with a small number of parameters, which reduces training time, data and the costs for network evaluation in a simulation. The memory of the network and the coarse multigrid solutions provide a “guide” for the corrections. In [1] we have demonstrated the efficiency and generalizability of DNN-MG for variations of the 2D laminar flow around an obstacle. DNN-MG improved the solutions as well as lift and drag functionals while requiring less than half the computation time of a full multigrid solution [3].

Although DNN-MG provides solutions with high accuracy and is computationally highly efficient in 2D, it is unclear how the method scales to 3D, where the computational effort is still a critical factor and the flow is much more complex. We investigate the scaling of DNN-MG to 3D flows. We also address the separation between testing and training time which includes data generation by employing an online learning approach and give an outlook on ways to incorporate unsupervised learning into the method.

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FE Approximation of Dirichlet Control Problems Governed by the Stokes System

Mariano Mateos¹

Control of fluids governed by the Stokes or Navier-Stokes equations is a question of major interest that has undergone a great development in the last years. We look for a velocity \mathbf{y} that minimizes the distance in L^2 to a prescribed target \mathbf{y}_d . To obtain \mathbf{y} , we can only control \mathbf{u} , its trace on the boundary of the domain, i.e., we want to solve

$$\min_{\mathbf{u} \in \mathbf{U}} \frac{1}{2} \|\mathbf{y}_{\mathbf{u}} - \mathbf{y}_d\|_{L^2(\Omega)}^2 + \text{regularization term}$$

subject to

$$-\Delta \mathbf{y}_{\mathbf{u}} + \nabla p = 0 \text{ in } \Omega, \quad \nabla \cdot \mathbf{y}_{\mathbf{u}} = 0 \text{ in } \Omega, \quad \mathbf{y}_{\mathbf{u}} = \mathbf{u} \text{ on } \Gamma, \quad \int_{\Omega} p = 0,$$

where $\mathbf{U} \subset L^2(\Gamma)$.

After giving a precise notion of solution in the transposition sense of the Stokes problem with Dirichlet data in Sobolev spaces with negative exponent, that will allow us to obtain optimal regularity results on polygonal domains, we will investigate three different kinds of regularization terms: usual L^2 regularization, energy-space regularization and tangential control. We will show that the optimal solutions satisfy different regularity properties and these properties will give an upper bound in the order of convergence we can obtain from finite-dimensional approximations.

Next, we will focus in the discretization of the tangential-control problem using hybridizable discontinuous Galerkin methods, HDG. To do this, a proper mixed formulation that includes the flux of the velocity $\mathbb{L} = \nabla \mathbf{y}$ must be used. This represents a problem, since, for Dirichlet data in $L^2(\Gamma)$, this flux is not a function. Moreover, for stabilization, the trace in the interior faces of the elements must be used. Thanks to our regularity results we are able to show that the flux is a function.

We will introduce two HDG formulations. First, a non-pressure-robust formulation that is able to deal even with what we call the “low-regularity” case, i.e., $\mathbf{y} \in \mathbf{H}^s(\Omega)$ for $s > 1$ and the trace of the flux may not be well defined. Second, we will show a pressure-robust variant. In this case, we can only treat the “high-regularity” case: $\mathbf{y} \in \mathbf{H}^s(\Omega)$ for $s > 3/2$ and the trace of the flux is well defined. At the price of a slightly higher computational cost, we can get, for the approximation of the velocity \mathbf{y} , error estimates which are independent of the size of the pressure.

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Some aspects of variational time discretisations of higher order and higher regularity

Gunar Matthies¹ Simon Becher²

As generalisation of the well-known discontinuous Galerkin (dG) and continuous Galerkin-Petrov (cGP) methods, a two-parametric family of variational time discretisations has been proposed recently. The two family parameters allow to control ansatz order and global smoothness of discrete solutions. Hence, higher order schemes with higher order regularity can be obtained by adjusting the family parameters in the right way.

Many variational time discretisation methods provide post-processing mechanisms leading to discrete solutions that converge in integral-based norms of one order higher than those of the original methods. In dependence of the two family parameters of the variational time discretisation schemes, we discuss two types of post-processing and study the influence of cascadic interpolation.

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Using structured multigrid methods in unstructured FEM solvers

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Multigrid methods have been developed for both structured and unstructured grids. Due to their purely algebraic construction of coarse levels, algebraic multigrid (AMG) methods are particularly appealing for unstructured grid scenarios. Yet, they come with considerable setup cost due to indirect indexing into matrices defined on unstructured grids as well as communication on parallel machines, since many operations (foremost the Galerkin product RAP) require communication among data structures defined on the entire mesh. In contrast, hierarchical hybrid grids (HHGs) apply local grid refinement to benefit from structured grid performance, however cannot be interfaced with mature application codes in a straightforward manner [1].

In [2], we propose a non-invasive multigrid method that combines the idea of AMG and HHG: while grid structure in some localized parts of the mesh allows for efficient structured grid algorithms, a hierarchy of coarse levels is formed in a purely algebraic fashion. This solver, named Region MG, can easily be used with existing application codes and allows to leverage structured multigrid components for partially structured meshes without re-implementing the discretization and matrix assembly procedure. Based on minimal user-provided meshing information, the multigrid hierarchy can be defined purely locally. Communication among processes is only required during an initial pre-processing of the input matrix as well as after restriction to a coarser level. Foremost, the Galerkin product RAP can be formed without any parallel communication.

In this presentation, we will develop a mathematical framework underpinning the proposed Region MG method for partially structured grids. We will show its equivalence to established AMG solvers as well as its performance benefits. We will apply Region MG to hypersonic flow problems and demonstrate its superiority over more traditional AMG preconditioners.

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Local convergence of the FEM for the integral fractional Laplacian

Jens Markus Melenk¹ Markus Faustmann² Michael Karkulik³

For first order discretizations of the integral fractional Laplacian we provide sharp local error estimates on proper subdomains in both the local H^1 -norm and the localized energy norm. Our estimates have the form of a local best approximation error plus a global error measured in a weaker norm.

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A priori and a posteriori error analysis for a hybrid formulation of a prestressed shell model

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This work deals with the finite element approximation of a prestressed shell model in the case of isometrically deformed shell. Using a new formulation where the unknowns (the displacement and the rotation of fibers normal to the midsurface) are described in Cartesian and local covariant basis respectively. Due to the constraint involved in the definition of the functional space, a penalized version is then considered. We obtain a non robust a priori error estimate of this penalized formulation, but a robust one is obtained for its mixed formulation. Moreover, we present a reliable and efficient a posteriori error estimator of the penalized formulation. Numerical tests are included that confirm the efficiency of our residual a posteriori estimator.

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Reduced order modelling using neural networks for predictive modelling of 3D-magneto-mechanical problems with application to magnetic resonance imaging scanners

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The design of magnets for Magnetic Resonance Imaging (MRI) scanner requires requires multiple parameters and loading conditions to be investigated to aid with design and the manufacturing process. The coupled physical processes involved mean that a 3D magneto mechanical problem must be simulated where parameters, such as the excitation frequency and electric conductivity, are varied. Full order model simulations using finite elements require fine discretisations using dense meshes and/or high order elements and so can take up a significant amount of time and resources within the design process and, thus, can be costly. Previous work by our group has focused on the application of Proper Orthogonal Decomposition (POD) Reduced Order Models (ROM), but this has a highly invasive computational implementation. With the further coupling of additional physics in mind, alternative approached based on neural network based ROMs will be presented. In the talk, we will compare the performance of several different such ROMs for predicting the magneto-mechanical coupled simulations in both the frequency and shield conductivity parameter space using a test magnet configuration. We will conclude with some future work which include the efficient and accurate simulation of quench inside an MRI magnet with the use of machine learning for prediction.

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A priori and a posteriori error estimates for the Deep Ritz method applied to the Laplace and Stokes problem

Piotr Minakowski¹ Thomas Richter²

We analyze neural network solutions to partial differential equations obtained with Physics Informed Neural Networks. In particular, we apply tools of classical finite element error analysis to obtain conclusions about the error of the Deep Ritz method applied to the Laplace and the Stokes equations. Further, we develop an a posteriori error estimator for neural network approximations of partial differential equations. The proposed approach is based on the dual weighted residual estimator. It is destined to serve as a stopping criterion that guarantees the accuracy of the solution independently of the design of the neural network training. The result is equipped with computational examples for Laplace and Stokes problems.

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A Finite element method for solving 2D contact electro-elastic antiplane with friction

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In this work, we describe a numerical method for 2D non-smooth contact problems with Tresca friction. First, we study the antiplane frictional contact models for electro-elastic materials. The material is assumed to be electro-elastic and the friction is modeled with Tresca's law and the foundation is assumed to be electrically conductive. First we establish the existence of a unique weak solution for the model. Moreover, the Proof is based on arguments of evolutionary inequalities. Comparison is made with results obtained using a finite element program, ANSYS. Selected numerical examples of application of the algorithm are presented here.

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A high-order FEM for distributed-order subdiffusion equations

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We consider the following distributed-order time-fractional diffusion, subdiffusion, equation

$$\begin{cases} \mathfrak{D}_t^\omega u - \Delta u = f(\mathbf{x}, t), & \forall (\mathbf{x}, t) \in \Omega \times (0, T], \\ u(\cdot, t)|_{\partial\Omega} = 0, \quad t \in [0, T]; \quad u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \end{cases}$$

where $\Omega \in \mathbb{R}^2$ is a bounded Lipschitz domain and \mathfrak{D}_t^ω is the distributed-order fractional derivative, defined by

$$\mathfrak{D}_t^\omega u(\cdot, t) = \int_0^\beta \omega(\alpha) \mathcal{D}_t^\alpha u(\cdot, t) d\alpha, \quad 0 < \beta \leq 1,$$

in which $\omega(\alpha) \geq 0$, $\int_0^\beta \omega(\alpha) d\alpha = c_0 > 0$ and \mathcal{D}_t^α denotes the Caputo fractional derivative of order $\alpha \in (0, 1)$ which is defined as $\mathcal{D}_t^\alpha u(\cdot, t) = (1/\Gamma(1 - \alpha)) \int_0^t (t - s)^{-\alpha} u_t(\cdot, s) ds$. The time-fractional distributed-order derivative is in fact a continuous generalization of the single-order time-fractional one, i.e. setting the single Dirac- δ function as ω leads to the ordinary time-fractional derivative. Hence, an effective numerical method for the distributed-order subdiffusion equation is necessary to develop. Utilizing the proposed formula by Mokhtari and Mostajeran, called L1-2-3, to approximate the distributed-order derivative and applying a finite element method (FEM) for spatial discretization, we develop a high temporal order fully discrete scheme. Combining with the idea of analysing the L1-2-3 FEM for the subdiffusion problem extended by Ramezani et al., we establish stability and convergence analyses of the proposed scheme. Detailed analysis indicates that the proposed L1-2-3 FEM is unconditionally stable and convergent with the convergence order $O(\tau^{4-\beta} |\ln \tau|^{-1} + h^2 + h_\alpha^2)$, where τ , h , and h_α are the step size in time, space, and distributed-order, respectively. The important point to note here is the improving the temporal convergence rate compare with the investigated method by Huang et al. in solving the distributed-order subdiffusion equation. Finally, some numerical examples are presented to support the theoretical prediction.

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Discontinuous Galerkin Isogeometric Analysis for some elliptic problems with Singularities

Stephen Moore¹

Multipatch discontinuous Galerkin Isogeometric Analysis (dGIGA) consists of decomposing complex domains into several subdomains usually called patches. Many real-life engineering applications also involve complex domains with non-smooth boundary parts, changing boundary conditions, non-smooth coefficients arising from material interface, etc. It is well known that standard numerical schemes on uniform meshes do not yield optimal convergence rate due to the regularity of the solution in the vicinity where the singularities occur. We therefore develop and analyze a graded mesh for multipatch discontinuous Galerkin isogeometric analysis (dGIGA) which leads to the desired and expected optimal convergence rate. The dGIGA mesh grading uses a priori information of the behavior of the solution around the points, where the singularity occurs, and create an appropriate mesh sequence yielding the same convergence rate as in the smooth case. In this talk, we present a priori error estimates and numerical results for non-matching meshes along the patch interfaces.

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On a deep neural network algorithm for solving backward heat conduction problems

Farinaz Mostajeran¹ Reza Mokhtari²

In recent years, due to wide applicability, straightforward implementation, and great performance in practice, there is an interest in applying the artificial neural network (ANN), or simply neural network (NN), strategy to solve numerous inverse problems in many disciplines. Partial differential equations (PDEs) used to model real-world problems are one category that researchers try to solve by employing neural networks to eliminate the loss of numerical discretization and avoid mesh generation. Recently, the idea of solving forward and inverse PDEs with deep neural networks was proposed in by Raissi et al. These networks are referred to as physics-informed neural networks (PINNs). The reason behind the success of PINNs is relying on well-developed tools such as automatic differentiation for dealing with partial differential terms. Moreover, neural network models are good approximators for high-dimensional functions that can be trained efficiently in most cases. Mostajeran and Mokhtari applied PINNs to solve backward heat conduction problems (BHCPs), which have been long-standing computational challenges due to being ill-posed. The primary benefit of this method is overcoming the complexity of the domain with various boundary conditions. Without needing any discretization of the time or space, the algorithm can retrieve the unknown solution on the domain if given a sufficient number of sampled training data. This revolutionary strategy can efficiently and accurately extract the pattern of the solutions even when the noise corruption of up to ten percent is imposed on input data. Moreover, when the final time is increased further, this approach is efficient in recovering the data at the initial time, which accentuates the method's robustness. We also show that there exists a neural network such that the corresponding loss function converges to zero. Furthermore, we prove that this neural network strongly converges to the final solution on the domain and weakly converges to the solution of the BHCP over its domain at each time.

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Formation of wrinkles in bi-layer systems

Lisa Julia Nebel¹

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

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

in the admissible set

$$\mathcal{A} = \left\{ (\varphi, R) \in W^{1,q}(\Omega, \mathbb{R}^3) \times H^1(\Gamma_c, \text{SO}(3)) \mid \begin{array}{l} \varphi \text{ is a deformation function,} \\ (\varphi, R) \text{ fulfill the Dirichlet boundary conditions} \end{array} \right\}$$

with $q > 3$. We discretize the problem using Lagrange finite elements for the substrate displacement and geodesic finite elements for the microrotation field. Geodesic finite elements are a generalization of standard finite elements to spaces of functions mapping to a Riemannian manifold. We prove the existence of solutions of the discrete coupled model.

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

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Error analysis for a moving boundary problem describing the penetration of a diffusant concentration into rubbers

Surendra Nepal¹

We propose a moving-boundary scenario to model the penetration of diffusants into rubbers. Immobilizing the moving boundary by using the well-known Landau transformation transforms the original governing equations into new equations posed in a fixed domain. We solve the transformed equations by the finite element method. Numerical simulation results show that the computed penetration depths of the diffusant concentration are within the range of experimental measurements. To have trust in the obtained simulation results, we perform the numerical analysis for our setting. Initially, we study semi-discrete finite element approximations of the corresponding weak solutions. We prove both a priori and a posteriori error estimates for the mass concentration of the diffusants, and respectively, for the a priori unknown position of the moving boundary. Finally, we present a fully discrete scheme for the numerical approximation of model equations. Our scheme is based on the Galerkin finite element method for the space discretization combined with the backward Euler method for time discretization. In addition to proving the existence and uniqueness of a solution to the fully discrete problem, we also derive a priori error estimates for the mass concentration of the diffusants, and respectively, for the position of the moving boundary. Our numerical illustrations verify the obtained theoretical order of convergence in physical parameter regimes.

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An analysis of high-frequency Helmholtz problems in domains with conical points and their finite element discretization

Serge Nicaise¹ Théophile Chaumont-Frelet²

We consider Helmholtz problems in three-dimensional domains featuring conical points. We focus on the high-frequency regime and derive novel sharp upper-bounds for the stress intensity factors of the singularities associated with the conical points. We then employ these new estimates to analyze the stability of finite element discretizations. Our key result is that lowest-order Lagrange finite elements are stable under the assumption that " $\omega^2 h$ is small". This assumption is standard and well-known in the case of smooth domains, and we show that it naturally extends to domain with conical points, even when using uniform meshes.

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Existence and Uniqueness for some Non-Resonant Quasilinear Elliptic Systems with Variable Exponents

Anass Ouannasser¹

In this paper, we study the solvability to the left of the first eigenvalue for some non-resonant quasilinear elliptic problems involving variable exponents. We first prove the existence of at least a weak solution for some non-variational systems by using a surjectivity result for pseudomonotone operators. Furthermore, under additional conditions, we show that the solution is unique. Secondly, we deal with non-resonant related equations and obtain existence and uniqueness results by using a variational approach.

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A 3D finite element - boundary element coupling method in time domain

Ceyhun Özdemir¹ Heiko Gimperlein² Ernst Peter Stephan³

We consider a transmission problem, where the homogeneous wave equation on a bounded Lipschitz domain Ω is coupled with another homogeneous wave equation on the exterior $\Omega^c = \mathbb{R}^3 \setminus \Omega$. We derive a variational formulation based on the Poincare-Steklov operator. We use a tensor product ansatz and derive an efficient time stepping scheme, precisely the Marching-on-in time (MOT) scheme. Finally, we conclude the presentation with different numerical examples.

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Simulating the seismic ground motion impact on large buildings: A 3D-1D Finite Element-Truss Model coupling

Amir Peiraviminaei¹ Barbara Wohlmuth² Markus Muhr³ Marco Stupazzini⁴ Ilario Mazzieri⁵

In this presentation, we consider one-directionally coupled 1D structures with a 3D ground motion. THE 3D Elastodynamic problem is considered for ground motion caused by earthquakes which triggers shaking in structures like high-rise buildings and bridges. Due to the population growth, the need for accommodation has led to constructing high-rise buildings and very dense Megacities. Finite Element Analysis of the dynamic displacement and motion of these structures have been studied thoroughly, in which, 3D models for the building layouts are fully integrated into the geological ground structure. We want to use 1D multi degree of freedom oscillators to represent the structures instead and study a one directional coupling of soil structure interaction. This approach is very cost efficient to implement. By increasing the amount of DoFs for any urban structure, we can simulate more realistically the impact of seismic events on whole city districts while simulation costs remain mostly at the order of the ground motion simulation alone. For this purpose, we consider first a very simple 3 DoF model with a prescribed analytical solution. After validating our Algorithm, we consider an MDoF model for a city-like environment and a bridge which are exposed to an earthquake considering A linear constitutive material law.

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Finite element error estimates for PDEs with irregular Dirichlet boundary data using boundary concentrated meshes

Johannes Pfefferer¹ Max Winkler²

This talk is concerned with finite element error estimates for PDEs with inhomogeneous Dirichlet boundary data in convex polygonal domains. The Dirichlet boundary data are assumed to be irregular such that the solution of the PDE does not belong to $H^2(\Omega)$ but only to $H^t(\Omega)$ for some $t \in (1, 2)$. As a consequence, a discretization of the PDE with linear finite elements exhibits a reduced rate in $L^2(\Omega)$ and $H^1(\Omega)$. In order to restore the best possible convergence rate we propose and analyze in detail the usage of boundary concentrated meshes. These meshes are gradually refined towards the whole boundary. The corresponding grading parameter does not only depend on the regularity of the Dirichlet boundary datum but also on the norm, which is used to measure the error. That means, different grading conditions are necessary for the error in $L^2(\Omega)$ and $H^1(\Omega)$. In numerical experiments we confirm the behavior predicted by our analysis.

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Space-Time Enriched Finite Element Methods for the Wave Equation

Kieran Quaine¹ Heiko Gimperlein²

Generalised finite elements based on plane-wave enrichments have been shown since the late 1990s to significantly reduce the computational cost for the numerical approximation of wave emission and scattering problems in the frequency domain. The enrichment of the approximation space allows good approximation of the highly oscillatory solutions even on coarse mesh grids. We propose and investigate a generalized finite element method for the time-dependent wave equation based on enriching the approximation space by travelling plane waves. Our approach is based on a first-order discontinuous Galerkin formulation for the wave equation, discretised with continuous elements in space and discontinuous elements in time. We build on recent progress using time-independent enrichments, which is limited by the small time steps required for solutions involving high frequencies. The space-time enrichment in this work achieves good approximation for coarse spatial meshes and large time steps, with a corresponding reduction in computational effort. Numerical results indicate the advantages of the proposed approach and investigate the attained accuracy of our scheme as the number of enrichment functions is increased.

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A local discontinuous Galerkin method for the subdiffusion inverse source problem with a weakly singular solution

Mohadese Ramezani¹ Reza Mokhtari²

In this talk, the aim is to determine the source term in an inverse problem corresponding to the following time-fractional diffusion, subdiffusion, equation

$$\begin{cases} \mathcal{D}_t^\alpha u - \Delta u = f(x)p(t), & (x, t) \in \Omega \times (0, T], \\ u(\cdot, t)|_{\partial\Omega} = g(t), \quad t \in [0, T]; \quad u(x, 0) = u_0(x), \quad x \in \Omega, \end{cases}$$

where u and f or p are unknown functions, and \mathcal{D}_t^α stands for the Caputo fractional derivative of order $\alpha \in (0, 1)$, i.e. $\mathcal{D}_t^\alpha u(\cdot, t) = (1/\Gamma(1 - \alpha)) \int_0^t (t - s)^{-\alpha} u_t(\cdot, s) ds$. To solve the inverse problem, we need one of the following over-specified conditions

$$\begin{aligned} u(x, T) &= h_1(x), & x \in \Omega, \\ u(x^*, t) &= h_2(t), & t \in [0, T], \quad x^* \in \Omega. \end{aligned}$$

The time-fractional diffusion problems taking into consideration Caputo fractional derivative usually have singular solutions near the initial time, i.e. $t = 0$. In this case, numerical methods generated on the uniform mesh break down in facing the problem and adaptive mesh refinement is needed near the initial time to hold the convergence order. Yeganeh et al. proposed a method based on the well-known L1 formula and the local discontinuous Galerkin (LDG) scheme to determine the space-dependent source term. Here, we consider both space- and time-dependent source determination in the inverse problem with a weakly singular solution.

We extend a method based on the L1-2-3 formula, proposed by Mokhtari and Mostajeran, for approximating the Caputo derivative and a local discontinuous Galerkin method in the spatial direction. The L1-2-3 approximation is used on a mesh that is graded in time, taking into account the initial singularity of the solution. It is indicated that the convergence order of the proposed graded L1-2-3 LDG method is $\mathcal{O}(N^{\min\{r, 3\}})$ while the convergence order of methods used uniform meshes is reduced. Finally, numerical results show the effect of the adaptively graded mesh on the convergence order of the proposed method.

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Fluid-rigid body interactions with large motion and contact

Thomas Richter¹ Martyna Minakowska² Henry von Wahl³

We consider a simple problem: a solid, e.g. a sphere, is falling towards the bottom in a container filled with a liquid. First, we present efficient simulation methods that cope with this large-displacement problem. The fundamental problem is that the solid is moving substantially and therefore the flow domain undergoes strong changes. This situation is difficult to grasp numerically. We introduce different modeling and discretization approaches, both classical ones and those that are based on neural networks to depict the forces between fluid and solid. We present numerical benchmarks, which are also backed by experimental data.

Then we deal with the contact of the solid with the bottom of the container. Analytically this problem is already well studied and here the unpleasant result is that contact in finite time is not possible if the fluid will be assumed to be incompressible. In reality, however, we will find that the ball bounces off the ground and comes to rest only after a few contacts.

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Mortar coupling of hp-discontinuous Galerkin and boundary element methods for the Helmholtz equation

Alexander Rieder¹ Christoph Erath² Lorenzo Mascotto³ Jens Markus Melenk⁴ Ilaria Perugia⁵

In this talk, we present a way to couple a discontinuous Galerkin method with a boundary element method to solve the Helmholtz equation with variable coefficients. The focus is on the case of high wavenumbers. The coupling is realized with a mortar variable that is related to an impedance trace on a smooth interface. We prove wavenumber explicit quasi-optimality of the *hp*-version of the scheme, under a weak threshold condition on the approximability properties of the discrete spaces. The key ingredients are a novel discontinuous-to-continuous reconstruction operator on tetrahedral meshes with curved faces and a careful wavenumber explicit regularity analysis of the adjoint problem.

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Computational Bite Force Estimation from a Human Mandible Density Profile

Hazim Saleh¹

Introduction Occlusal overload of dental implants produces complications which may result in its failure. While bite force information is essential to properly design and position dental implants, it is not routinely available. According to Julius Wolff bone morphology is a product of its loading history [1], we investigate the possibility of extracting bite force information from a human mandible geometry and its corresponding density map (CBCT images).

Methods We first build a forward model by adopting and expanding on the theory which treats bone as a self optimizing material and remodels till reaching a fixed value of natural strain energy density introduced by Huiskes [2]. The computer model is based on the finite element method (FEM), we assume the bone domain is occupied by a linear elastic continuum where it's mechanical properties are dependent on it's apparent density. Given an initial state, we apply bite forces on a human mandible geometry producing a strain energy signal. We assume the signal diffuses to the surrounding tissue and decays at a constant rate described by the diffusion equation. We assume this process to be fast and therefore to be in a stationary state. Secondly, we use the developed model to generate pairs of bite forces and density profiles, the problem is solved in an inverse setting using a least squares FE approximation.

Results The proposed forward bone remodeling sensory model doesn't suffer from stiffness localization while being suitable for large meshes and 3D applications.

Conclusion Here, we propose an extended forward model for bone remodeling. Undergoing work is focused on identifying bite forces from the generated density. Future work will include validating the model.

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High order Crouzeix-Raviart elements in two- and higher dimension.

Stefan Sauter¹

In our talk we present Crouzeix-Raviart elements of general polynomial degree k in two and higher dimension. We employ this space for the velocity discretization of the Stokes problem while the pressure is discretized by discontinuous polynomials of degree $k-1$. We prove estimates of the discrete inf-sup constant which are explicit in k and the mesh width h and report on progress in higher dimension

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Matrix-valued Finite Elements with Applications in Mechanics and Curvature Computation

Joachim Schöberl¹

We present matrix-valued finite element spaces and discuss canonical differential operators and duality pairings. We demonstrate good approximation properties of the methods in applications from solid and structural mechanics, fluid dynamics, and computation of curvature.

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Supremum-norm a posteriori Error Control of Quadratic Discontinuous Galerkin Methods for the Obstacle Problem

Ritesh Singla¹ Rohit Khandelwal² Kamana Porwal³

Elliptic obstacle problem is a prototype model for the class of elliptic variational inequalities of the first kind. It is a nonlinear model that describes the vertical movement of an object restricted to lie above a barrier (obstacle) while subjected to a vertical force (with suitable boundary conditions). In this talk, we are going to discuss about *a posteriori* error analysis in the supremum norm for the quadratic Discontinuous Galerkin(DG) method for the elliptic obstacle problem. In comparison with the energy norm estimates, supremum norm estimates gives the pointwise control on the error. We have carried out the analysis on two different discrete sets, one set having integral constraints and other one with the nodal constraints at the quadrature points, and discuss the pointwise reliability and efficiency of the proposed a posteriori error estimator. In the analysis, we employ a linear averaging function to transfer DG finite element space to standard conforming finite element space and exploit the sharp bounds on the Green's function of the Poisson's problem. Moreover, the upper and the lower barrier functions corresponding to continuous solution u are constructed by modifying the conforming part of the discrete solution u_h appropriately. The analysis is carried out in a unified setting which holds for several DG methods. Finally, the numerical results for adaptive FEM are presented in order to exhibit the reliability and the efficiency of the proposed error estimator.

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Towards the design of an in-silico computational tool for the simulation of floorborne vibrations on magnetic resonance imaging scanners

Yashwanth Sooriyakanthan¹ Antonio Gil² Paul Ledger³ Mike Mallett⁴

The in-silico simulation of the effects of vibration on Magnetic Resonance Imaging (MRI) scanners is currently not possible within an industrially viable timeline (source: Siemens Healthineers). Specifically, existing three-dimensional transient solvers for coupled magneto-mechanics are not compatible due to their extremely high computational cost, thus requiring a new computational approach. Within an MRI scanner, the effects of gradient Alternating Current (AC) coils can be safely superimposed over those of superconducting Direct Current (DC) coils due to their very different orders of magnitude, permitting to leverage an efficient linearised frequency-based approach which can be effectively used during the MRI design phase.

Previous work by our group [1, 2, 3] focused on the development of a computational framework where a Lagrangian formulation was used to describe the magneto-mechanical problem of interest. After derivation of the weak form and linearisation, hierarchical H1 and H(curl) conforming finite element basis functions were used to discretise the displacement and vector potential fields of the magneto-mechanical problem of interest, respectively. Thus far, the effect of potential floor-borne vibrations has been disregarded, that is, the movement of the conducting shields was restricted to zero. In this poster, we will further expand our previous framework by exploring the effect that floor-borne vibrations can have on some of the fields of interest, specifically, the generation of eddy currents, ohmic power and kinetic energy. This will be achieved by relaxing the above homogeneous Dirichlet constraint on conductors and permitting the consideration of more complex vibration modes. The focus of future work, in collaboration with Siemens Healthineers, will be the accurate simulation of any field perturbation (linking it to MRI imaging) as a result of possible floor-borne vibrations in both MRI conducting shields and coils.

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Multirate Adaptive Time-stepping Schemes for Coupled Systems of PDEs

Martyna Soszynska¹ Thomas Richter²

We study time discretization schemes for coupled systems of partial differential equations. We assume that the subproblems are defined over spatially distinct domains with a common interface, where the coupling is enforced. Each of the physical problems can be governed by a different type of equations (either parabolic or hyperbolic) and therefore can exhibit different dynamics. Fluid-structure interactions are one type of important application problems that fall into this framework. Here however, we will consider linear problems only.

Our aim is to develop time discretization schemes allowing for different time-step sizes in each of the domains without violating the coupling conditions. We are able to achieve it by formulating the problems within the space-time framework. Although the formulation is monolithic, we solve the systems sequentially relying on a partitioned approach. We further develop an a posteriori error estimator based on the dual weighted residual method. This estimator is then used as an adaptivity criterion. To justify this method, we show stability estimates.

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Regularization and finite element error estimates for distributed control problems with energy regularization

Olaf Steinbach¹

In this talk we present a general concept for distributed optimal control problems with energy regularizations. Applications include the Poisson equation, the heat equation, and the wave equation. We derive error estimates between the state and the target with respect to the regularization parameter, and in combination with finite element error estimates we end up with an optimal choice for the relaxation parameter. Numerical examples are given.

This talk is based on joint work with U. Langer, H. Yang, and R. Löscher.

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On numerical simulation of FSI and FSAI models of human phonation by FEM

Petr Sváček¹

Recently, the numerical solution of FSI problems becomes both components of important also in biomechanics, among others in speech modeling. The numerical analysis of this case is very complicated: Human voice is created by passage of air flow between vocal folds, where the constriction formed by the vocal folds induces acceleration of the flow and vocal fold oscillations, which generates the sound. The modelling of such a complex phenomenon encounters many difficulties as it is a result of coupling complex fluid dynamics and structural behavior. In particular one needs to address the nonlinear coupled problems of fluid-structure (FSI) interactions. This is realized by using the mathematical description of a relevant problem and its numerical approximation by the (stabilized) finite element method. This includes the discretization of the elasticity equations describing the motion of an elastic structure and the air flow modelled by the Navier-Stokes equations. Both models are coupled via interface conditions. The approximation of flow in moving domains is treated with the aid of the Arbitrary Lagrangian-Eulerian method. The incompressible Navier-Stokes equations are approximated by the stabilized finite element method. The time discretization based on a semi-implicit linearized scheme is described and the solution of the coupled problem of fluid-structure interaction is realized by a coupling algorithm. The aeroacoustics is treated using the so called hybrid approach, where either the Lighthill's approach is used to address the acoustic problem. The numerical results are shown.

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Numerical Modelling of Temperature-based Time of Death Estimation

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Gita Mall⁶

In forensic medicine, up to now the time of death is estimated based on a single measurement in the body core. To yield higher accuracy than established phenomenological models and take all relevant cooling mechanisms into account, we can simulate the thermodynamic heat transfer on a meshed corpse by a finite element (FE) based method. We then solve a regularized inverse problem to identify parameters by a gradient-based method to minimize the model-data mismatch. For this, besides the availability of human phantoms, highly detailed anatomical models with organs and tissue types have been segmented and reconstructed from CT scans of corpses. Implementation of this model is carried out within the FE toolbox Kaskade 7. Here, the body is represented by a spatial grid of tetrahedra and the temperature distribution at each time point is approximated by the temperature values at the grid nodes. The calculation of the cooling curves is then carried out by an implicit time-stepping method. We investigate the influence of heat transfer mechanisms like convection and radiation on the boundary and the impact of parameter variations and different measurement positions to get a qualitative understanding of relevance of thermal processes and modelling options for a sufficient accuracy of time of death estimation.

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Numerical Analysis of optimal control problem governed by transient Stokes equations with state constraints pointwise in time

Boris Vexler¹ Dmitriy Leykekhman²

We consider the following optimal control problem:

$$\text{Minimize } \frac{1}{2} \int_0^T \int_{\Omega} (u(t, x) - u_d(t, x))^2 dx dt + \frac{\alpha}{2} \int_0^T \int_{\Omega} q(t, x)^2 dx dt$$

subject to transient Stokes equations

$$\begin{aligned} \partial_t u - \Delta u + \nabla p &= q && \text{in } (0, T) \times \Omega \\ \nabla \cdot u &= 0 && \text{in } (0, T) \times \Omega \\ u &= 0 && \text{on } (0, T) \times \partial\Omega \\ u(0) &= u_0 && \text{in } \Omega \end{aligned}$$

and to state constraints formulated pointwise in time, i.e.

$$\int_{\Omega} u(t, x) \cdot w(x) dx \leq b \quad \text{for all } t \in [0, T]$$

with a given $u_d \in L^2(I; L^2(\Omega)^d)$ and $w \in L^2(\Omega)^d$. The domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ is assumed to be polygonal/polyhedral and convex.

The optimality system for this problem involves a Lagrange multiplier from the space of regular Borel measures $\mu \in \mathcal{M}([0, T])$, which affects the regularity of the solution. We discretize the problem with inf-sup stable finite elements in space and with a discontinuous Galerkin method in time. For this discretization we provide quasi-optimal error estimates for the state and the control. The analysis is based on recently established error estimates for the Stokes system [1].

References:

[1] N. Behringer, D. Leykekhman, B. Vexler: Fully discrete best approximation type estimates in $L^\infty(I; L^2(\Omega)^d)$ for finite element discretizations of the transient Stokes equations, *IMA Journal of Numerical Analysis* (2022).

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Adaptive quadratic finite element method for unilateral contact problem.

Tanvi Wadhawan¹

Numerical analysis of the non-linear problems arising from unilateral contact problems using finite element methods exhibits technical adversity both in approximating the continuous problem and numerical modeling of contact conditions on a part of the boundary. The Signorini contact model typically is a prototype model for the class of unilateral contact problem. The main aim of my talk is to present and analyze a posteriori error estimates in the energy norm of a quadratic finite element method for the frictionless unilateral contact problem which is modeled as elliptic variational inequality of the first kind. The major challenge involved using quadratic finite elements is to model the non penetration Signorini condition on the discrete solution along the contact region at both theoretical and numerical end. Compared to the linear finite elements, we compute more accurate discrete solution to unilateral contact variational inequalities using higher order finite elements. The reliability and the efficiency of a posteriori error estimator is discussed. The main idea in our analysis is the appropriate construction of the discrete counterpart of the continuous contact force density which helps in proving the main results of this article. The suitable decomposition of the discrete space V^h and a discrete space Q^h , where the discrete counterpart of the contact force density is defined, play crucial role in deriving a posteriori error estimates. The error estimator involves various residuals consisting the data of the problem, discrete solution and a Lagrange multiplier related to the obstacle constraint. The numerical results for adaptive FEM are presented in order to exhibit the reliability and the efficiency of the proposed error estimator.

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Fully Discrete Error Estimates for Finite Element Discretizations of the Instationary 2D Navier-Stokes Equations

Jakob Wagner¹ Boris Vexler²

We consider the instationary Navier-Stokes equations with homogeneous Dirichlet boundary conditions in a 2D domain Ω on a bounded time interval I . The equations are discretized in space by inf-sup stable pairs of finite element spaces, and in time via the discontinuous Galerkin method. This choice allows for a variational formulation of the discretized equations, which facilitates definition of dual equations, particularly useful for error estimates and the analysis of optimal control problems. We will derive an estimate of the error in the $L^\infty(I; L^2(\Omega))$ norm, which is of a best approximation-type and thus has optimal orders of convergence w.r.t. the spacial discretization parameter h and the time discretization parameter k . Under H^2 regularity assumptions and a right hand side in $L^\infty(I; L^2(\Omega))$ it is possible to relate this error estimate for the nonlinear Navier-Stokes equations to the corresponding error estimate for the linear Stokes equations, which was shown by Behringer, Vexler and Leykekhman (2022). Since the energy estimate for the solution to the Navier-Stokes equations provides a bound for the $L^2(I; H^1(\Omega))$ - and $L^\infty(I; L^2(\Omega))$ norms in a combined fashion, many error estimates treat the error in these two norms jointly. This results in a suboptimal rate of convergence with respect to the spacial discretization parameter h , due to the $H^1(\Omega)$ norm contribution. Since we estimate the error individually, we can make full use of the $L^2(\Omega)$ norm, allowing for an improved estimate.

References:

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Space-time discontinuous Galerkin methods for weak solutions of hyperbolic linear symmetric Friedrichs systems

Christian Wieners¹ Daniele Corallo² Willy Dörfler³

We study weak solutions and its approximation of hyperbolic linear symmetric Friedrichs systems describing acoustic, elastic, or electro-magnetic waves. Stability and convergence estimates are provided for a discontinuous Galerkin discretization in space and time with respect to a mesh-dependent DG norm, where we also consider the case of piecewise discontinuous weak solutions. A reliable error estimator is constructed, and numerical results demonstrate the efficiency of the approach.

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Optimization of pedestrian dynamics

Max Winkler¹

In this talk we investigate a PDE system modeling the dynamics of pedestrians in an emergency scenario. The model consists of a nonlinear transport equation and an Eikonal equation providing a potential which determines the movement direction of the individuals. Although people tend to optimize their own situation in a greedy way, this will not lead to an optimal evacuation of the whole crowd. As a remedy, we introduce agents which locally attract the people and aim at finding their optimal trajectories minimizing the evacuation time. The agent dynamics are modeled by an additional ODE.

We study existence and regularity of solutions of the coupled PDE-ODE system and derive necessary optimality conditions for the optimal control problem. For a numerical solution we investigate a discretization based on a finite volume method in space and a Runge-Kutta scheme in time such as gradient-based optimization methods.

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Isogeometric approximation of the eigenfrequencies of membranes with cracks and application to shape identification

Philipp Zilk¹ Thomas Apel²

The eigenfrequencies of a vibrating membrane generally depend on its shape. The associated inverse problem which became famous through the work of Kac has been widely discussed in the literature. We look at this problem in the context of cracks. Is it possible to identify a crack in a membrane when the eigenfrequencies are known? At current stage, we work with a model that is based on simulated eigenvalues, for which we need good quality simulations of vibrating membranes with cracks. Therefore we use Isogeometric Analysis (IGA) in combination with graded meshes. IGA produces better results than FEM for one-dimensional eigenvalue problems. Some two-dimensional comparisons will be shown in the talk. Mesh grading techniques help to recover the optimal convergence order despite existing singularities in the domain and have been proven effective for multipatch discontinuous Galerkin IGA schemes. We provide numerical examples to show the effectiveness of mesh grading for eigenvalue problems in a single patch IGA framework.

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