TECHNISCHE UNIVERSITÄT
CHEMNITZ

Fakultät für Mathematik

Chemnitz FE-Symposium 2024

Chemnitz
FE
Symposium

Programme

Collection of abstracts

List of participants

Chemnitz, September 09 - 11, 2024

Scientific Topics:

The symposium is devoted to all aspects of finite elements and related methods for solving 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:

- Discontinuous Galerkin Methods,
- Shape Optimization,
- Pressure Robustness and Mass Conservation in Incompressible Flows.

Invited Speakers:

Susanne Brenner (Louisiana State University)
Jay Gopalakrishnan (Portland State University)
Michael Hinze (Universität Koblenz)

Sponsors:

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Th. Apel (München), F. Bertrand (Chemnitz), S. Beuchler (Hannover), O. Ernst (Chemnitz), G. Haase (Graz), H. Harbrecht (Basel), R. Herzog (Heidelberg), M. Jung (Dresden), U. Langer (Linz), A. Meyer (Chemnitz), O. Rheinbach (Freiberg), A. Rösch (Duisburg-Essen), O. Steinbach (Graz), M. Stoll (Chemnitz), M. Winkler (Chemnitz)

Organising Committee:

F. Bertrand, T. Dagli, A.-K. Glanzberg,
Z. Kassali, K. Seidel, M. Winkler

`www.chemnitz-am.de/cfem2024/`

Internet Access

The co56 hotel offers free internet access. Access details can be obtained from the reception.

Food

The conference fee includes:

- Lunch on all days of the symposium
- Dinner on Monday and Tuesday
- Tea and coffee during breaks

For participants staying at the co56 hotel there is a breakfast buffet.

Excursion and Social Program

On Monday, 17:00-19:00, we will have a tasting of specialities from the region of Saxony: oil, balsamic vinegar, wine and schnapps.

On Tuesday, 14:00-18:00, we will visit the ”Munzer Braumanufaktur” (Reichsstraße 1, 09112 Chemnitz), a small brewery in the city of Chemnitz. We will have a guided tour through the brewery and a beer tasting afterwards. We will meet at 14:00 in front of the co56 hotel and walk to the brewery.

Programme

Programme for Monday, September 9, 2024

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Collection of Abstracts

DD-LOD

Susanne Brenner[1]

DD-LOD is a multiscale finite element method for problems with rough coefficients that is based on a domain decomposition approach to the localized orthogonal decomposition methodology. I will present the construction and analysis of DD-LOD for elliptic boundary value problems with rough coefficients that only require basic knowledge of finite element methods, domain decomposition methods and numerical linear algebra. An application to elliptic optimal control problems will also be discussed.

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Domain Decomposition for Rotating Electrical Machines in Space-Time

Michael Reichelt[1] Sebastian Schöps[2]

Transient simulations of electrical machines are an important task in the design process of electrical machines. In classical time stepping schemes, the rotation is usually realized by distorting the mesh or by applying Mortaring. The former necessitates frequent remeshing and the latter careful choice of parameters. Another approach is to apply space-time finite element methods, where movement is already incorporated in the mesh. This is especially feasible when the movement is known in advance. In this talk we present a space-time finite element approach, where we make use of the special geometry of the two-dimensional model of an electrical machine and an analytic solution in the air gap. When using isogeometric analysis, and hence the exact geometry, this allows us to couple the air gap to fixed space- time meshes for the rotor and stator, even if the movement is not known in advance. Lastly, we give an outlook on how this approach can be extended to more general geometries.

References:

[1] https://graz.elsevierpure.com/en/publications/space-time-finite-element-methods-for-parabolic-problems

[2] https://arxiv.org/abs/2307.00278

[3] https://www.springerprofessional.de/en/on-the-stability-of-harmonic-coupling-methods-with-application-t/20213686

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phi-FEM: an optimally convergent finite element method on unfitted meshes

Alexei Lozinski[1] Michel Duprez[2] Vanessa Lleras[3] Killian Vuillemot[4]

We shall report on some new developments concerning ϕ-FEM – a fictitious domain finite element method. The method is well suited for elliptic and parabolic problems posed in domains given by smooth level-set functions without constructing a mesh fitting the boundary. ϕ-FEM achieves optimal convergence (attested both theoretically and numerically) using the finite elements of any order. Unlike other recent fictitious domain-type methods (XFEM, CutFEM), our approach does not need any non-standard numerical integration, neither on the cut mesh elements nor on the actual boundary. The main idea of ϕ-FEM is to extend the original problem slightly outside its domain (namely to the domain occupied by all the mesh cell having a non-empty intersection with the physical domain), and then write down a (formal) variational formulation on the extended domain using the level set to impose the boundary conditions ”implicitly” (either via a product of the levelset with the finite elements or by introducing auxiliary variables).

References:

[1] Duprez, M. and Lozinski, A. ϕ-FEM: a finite element method on domains defined by level-sets. SIAM J. Numer. Anal. 58 (2020) 2, pp. 1008-1028.

[2] Duprez, M. and Lozinski, A and Lleras, V. A new ϕ-FEM approach for problems with natural boundary conditions. Numer. Methods Partial Differ. Eq. 39 (2023) 1, pp. 281-303.

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Notes on session “Domain Decomposition (Küchwald 2-3)”

Matrix-valued Finite Elements for Solids, Structures and Fluids

Joachim Schöberl[1]

Vector-valued function spaces, their finite element sub-spaces, and relations between these spaces are well understood within the de Rham complex. The framework of differential forms and Hilbert complexes provides a unified framework for any space dimension. Various matrix-valued finite element spaces have been introduced and analyzed more or less independently. In this presentation we put these spaces into a so called 2-complex. We show applications in solid mechanics, plates and shell, curvature computation and fluid dynamics.

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Higher order discontinuous Galerkin methods in time and pressure-robust finite element discretizations applied to time-dependent generalized Stokes problems

Lukas Keller[1] Simon Becher[2] Gunar Matthies[3]

We consider discretizations of the time-dependent generalized Stokes equations based on pressure-robust inf-sup stable finite element methods in space and discontinuous Galerkin time-stepping schemes. Pressure robustness is ensured by using a reconstruction operator on the right-hand side, for the time derivative and in the reactive term. This ensures error estimates for the velocity that are completely independent of the pressure and, in particular, its smoothness. For a temporal interpolant of the right-hand side, we prove optimal convergence orders in space and time for both velocity and pressure. Furthermore, this temporal interpolant allows to perform two cheap post-processing steps in time that lead to an increased temporal accuracy, two orders for velocity and one order for pressure. Again, the velocity error constants are independent of the pressure. Numerical examples illustrate our theoretical results.

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Pressure-robustness in the context of the weakly compressible Navier–Stokes equations

Christian Merdon[1] Alexander Linke[2] Philip Lederer[3]

Pressure-robustness is an important property of a numerical scheme for accurate discretizations of the incompressible Navier–Stokes equations as it ensure the correct accounting of irrotational forces into the pressure gradient. For weakly compressible low Mach number flows the divergence-free part of the velocity is still large and is not affected by gradient forces. The talk connects pressure-robust discretizations for this divergence-free part with the well-balanced property for certain states like an atmosphere at rest where the pressure gradient balances the gravitational force.

Two families of methods that have this property are discussed. One employs a classical finite element method with an Hdiv-conforming interpolation in the right-hand side, the second directly employs Hdiv-conforming DG spaces. Together with a proper upwinding in the continuity equation at least their lowest order incarnations ensure density constraints and allow to show convergence on general shape-regular meshes. Numerical examples investigate convergence rates and illustrate the higher accuracy in well-balanced situations.

References:

[1] https://arxiv.org/abs/2311.06098

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Notes on session “Mixed Discretizations (Küchwald 2-3)”

Optimal Dirichlet Boundary Control Problems with Uncertain Data

Max Winkler[1] Hamdullah Yücel[2]

In this talk we study optimal Dirichlet boundary control problems where the diffusion coefficient, the source term and the boundary data in the state equation are uncertain. Existence of solutions and necessary optimality conditions are derived.

As solution algorithm we propose a stochastic Galerkin discretization. Special emphasis is put on preconditioning of the resulting linear systems and error estimates for the stochastic Galerkin discretization. Furthermore, we confirm the theoretical findings by numerical experiments.

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Numerical Analysis for Dirichlet Optimal Control Problems on Convex Polyhedral Domains

Johannes Pfefferer[1] Boris Vexler[2]

This presentation is concerned with the error analysis for finite element discretizations of Dirichlet boundary control problems. In contrast to most of the publications from the literature the underlying domain is assumed to be convex and polyhedral but not only polygonal. Optimal discretization error estimates are established in this case using the concept of variational discretization or using the approach of full discretization each based on standard linear finite elements. The convergence rates, which are proven, solely depend on the size of the largest interior edge angle. To be more precise, below the critical angle of $2\pi/3$, a convergence rate of one (times a log-factor) can be achieved for the discrete controls in the L^2-norm on the boundary. For larger interior edge angles the convergence rates are reduced depending on the size of this angle, which is due the impact of singular (domain dependent) terms in the solution. The results are comparable to those for the two dimensional case. However, the theoretical approaches from the two dimensional setting seem not to be directly extendable such that new techniques have to be used. At the end of the talk, the theoretical results are confirmed by numerical experiments.

References:

[1] https://arxiv.org/abs/2401.02399

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A unified finite element approach for PDE constrained optimal control problems

Olaf Steinbach[1] Ulrich Langer[2] Richard Löscher[3] Huidong Yang[4]

We consider an abstract frame work for the numerical solution of optimal control problems subject to partial differential equations. Examples include not only the distributed control of the Poisson equation, the heat equation, and the wave equation, but also boundary control problems. The approach covers the more standard L^2 setting, and the more recent energy regularization, also including state and control constraints. We discuss regularization and finite element error estimates and derive an optimal relation between the regularization parameter and finite element mesh size in order to balance the accuracy, and the costs. Finally we also discuss the efficient solution of the resulting (non)linear systems of algebraic equations. Numerical examples are given which confirm the theoretical findings.

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Notes on session “Optimal Control (Küchwald 1)”

Analysis of Divergence-Preserving Unfitted FEM for the Mixed Poisson Problem

Tim van Beeck[1] Christoph Lehrenfeld[2] Igor Voulis[3]

Geometrically unfitted finite element methods, e.g. CutFEM, XFEM, or unfitted DG methods, are popular modern tools for the numerical approximation of partial differential equations on complex or moving geometries, allowing the separation of the geometry description from the computational mesh. Commonly, these methods rely on stabilization techniques, for instance, ghost penalty (GP) stabilization, that ensure stability independent of the local cut configuration. Mixed finite element methods based on special vectorial finite element spaces, e.g. H(div)-conforming finite element spaces, however, are tailored to preserve conservation properties (e.g. mass conversation) exactly on the discrete level. While adding stabilization terms ensures the stability of the problem, the conservation properties are perturbed. In this talk, we introduce and analyze a stable discretization of the unfitted mixed Poisson problem with Dirichlet boundary conditions. Notably, our approach does not require stabilization terms that pollute the mass balance. The key idea is to formulate the divergence constraint on the active mesh instead of the physical domain, which yields a robust discretization independent of the cut configuration without the need for stabilization. This modification does not affect the accuracy of the flux variable and by applying postprocessing strategies to the scalar variable, we achieve optimal convergence rates for both variables and even superconvergence for the scalar variable.

References:

[1] https://arxiv.org/abs/2306.12722

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Numerical Analysis and Simulations of Fully Eulerian Fluid-Structure Interactions using Cut Finite Elements

Anne-Kathrin Wenske[1] Stefan Frei[2] Tobias Knoke[3] Marc C. Steinbach[4] Thomas Wick[5]

In this presentation, we discuss monolithic fluid-structure interactions in fully Eulerian coordinates using cut finite elements. The attractiveness of using Eulerian coordinates for the solid equations as opposed to arbitrary Lagrangian Eulerian approaches lies in the ability of the derived method to handle large deformations, topology changes and contact problems more easily. In such a setting the mesh is not fitted to the interface between the two physical subdomains as the interface is allowed to move freely through elements. For the treatment of cut elements we employ a CutFEM approach in the discretization, where the interface conditions are imposed weakly via Nitsche terms. It is well-known that the cuts impact the condition number of the resulting discrete systems such that additional stabilization is required. To this end, ghost penalty terms around the interface zone between the fluid and the solid are employed. In extension to the published literature, such a ghost penality approach for the entire fully Eulerian fluid-structure interaction problem is new. We establish theoretical results on quadrilateral elements for coercivity and inf-sub stability. The analysis is supplemented by some numerical examples with fixed interfaces.

References:

[1] https://arxiv.org/abs/2402.00209

[2] https://arxiv.org/abs/1605.09681

[3] https://doi.org/10.1016/j.apnum.2011.01.008

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Parameter-robust unfitted finite element methods for a Maxwell interface problem

Tim Haubold[1] Christoph Lehrenfeld[2]

Geometrically unfitted finite element methods such as CutFEM, Finite Cell, XFEM or unfitted DG methods have been developed and applied successfully in the last decades to a variety of problems, ranging from scalar PDEs on stationary domains to systems of PDEs on moving domains and PDEs on level set surfaces. These approaches combined with established tools of finite element methods allowed to apply and analyse unfitted methods in many fields. In this talk, we deal with an elliptic interface problem for the time-harmonic quasi-magnetostatic Maxwells equations.

Here the material function μ, the magnetic permeability, can jump at an interface. Such problems are considered in low-frequency applications. Standard unfitted Nitsche methods are not robust with respect to the parameter k, proportional to the wavenumber. For example, a standard Nitsche discretization for the curl-curl-operator introduces terms that do no longer vanish for gradient fields. In this talk, we will use a vectorial finite element discretization based on H(Curl) conforming functions. We will tackle the problem of robustness by using a mixed formulation and a Nitsche formulation. Additionally, we apply a careful tailored ghost penalization term.

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Notes on session “Interface Problems (Küchwald 4)”

Shape optimization with Lipschitz methods

Michael Hinze[1]

We present a general shape optimisation framework based on the method of mappings in the Lipschitz topology. We propose steepest descent and Newton-like minimisation algorithms for the numerical solution of the respective shape optimisation problems. Our work is built upon previous work of the authors in (Deckelnick, Herbert, and Hinze, ESAIM: COCV 28 (2022)), where a Lipschitz framework for star-shaped domains is proposed. To illustrate our approach we present a selection of PDE constrained shape optimisation problems and compare our findings to results from so far classical Hilbert space methods and recent p-approximations. We also provide numerical convergence analysis.

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Automatic shape optimization of non-linear multi-physics problems

Michael Gfrerer[1] Grégoire Allaire[2]

The Python package AutoFreeFEM [1] is developed for the purpose of automatic shape optimisation of non-linear multi-physics problems in FreeFEM++. Additionally, the package outputs expressions for use in LaTeX. As an input, the objective function and the weak form of the problem must be specified only once, ensuring consistency between the simulation code and its documentation. In particular, AutoFreeFEM provides the linearization of the state equation, the adjoint problem, the shape derivative, as well as a basic implementation of the level-set based mesh evolution method for shape optimization [2]. For the computation of shape derivatives, we utilize the Lagrangian approach for differentiating PDE-constrained shape functions. Differentiation is done symbolically using Sympy. In numerical experiments, we verify the accuracy of the computed derivatives. Finally, we demonstrate the capabilities of AutoFreeFEM by considering shape optimization of a non-linear diffusion problem, linear and non-linear elasticity problems, a thermo-elasticity problem and a fluid-structure interaction problem.

References:

[1] https://gitlab.tugraz.at/autofreefem/autofreefem

[2] Grégoire Allaire, Charles Dapogny, and Pascal Frey. Shape optimization with a level set based mesh evolution method. Computer Methods in Applied Mechanics and Engineering, 282:22–53, 2014.

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Equilibration-based a-posteriori error estimators for poro-elasticity

Maximilian Brodbeck[1]

Numerical solutions of poro-elasticity suffer from the deterioration of the overall accuracy when re-entrant corners, internal respectively boundary layers or shock-like fronts are present [1]. Estimates of the overall error, based on the numerical solution, offers a systematic way of retaining accuracy by localised mesh refinements. Following the seminal idea of Prager and Synge [2], such error estimates can be constructed based on the comparison of fluxes, directly calculated from the approximation, and any H(div) conforming function, satisfying the equilibrium condition. This function is typically called the equilibrated flux. More recently, this idea has been extended to linear-linear elasticity or the Biot equations [3,4]. Within this contribution we focus on the practice-relevant displacement-pressure formulation for quasi-static poro-elasticity. A space-time adaptive algorithm based on the equilibration of fluid flux and weakly symmetric stresses within the Raviart-Thomas finite element space is derived. Besides the efficiency of the error estimator algorithmic aspects of flux equilibration are discussed.

References:

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[2] W. Prager and J. L. Synge. "Approximations in elasticity based on the concept of function space". In: Quart. Appl. Math. 5 (1947), pp. 241–269.

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Iteratively Refined Image Reconstruction

Sebastian Neumayer[1] Mehrsa Pourya[2] Michael Unser[3]

On this poster, I discuss a framework for the learning of filter-based regularizers for image data. These can be deployed within a variational reconstruction ansatz for solving generic inverse imaging problems (universality of the regularizer). This ansatz ensures data consistency. Moreover, we are able to derive stability guarantees. Both are very important when working in critical applications such as medical imaging, since false diagnosis can have fatal consequences. Interestingly, the learned regularizers closely resemble traditional hand-crafted ones.

After introducing the baseline architecture, I will discuss a refinement of this architecture by conditioning the regularizer on the given measurements based on the initial reconstruction. This mechanism allows to compensate for the rather simple fields-of-experty architecture of the regularizer and adapts it to the actually observed measurements. By carefully designing the conditioning mechanism, we can preserve many of the favorable properties of the initial approach. In particular, learning the conditioning networks (which we will identify as strcture extractors) remains independent of the data. In the last part of the talk, I will present numerical results for denoising and MRI. These indicate that even relatively restricted architectures can achieve highly competitive performance.

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Mixed finite element for Stokes eigenvalue problem

Tugay Dagli[1] Fleurianne Bertrand[2]

In this talk, we present a novel three-field finite element for the Stokes eigenvalue problem. To this end, we approximate the Hellinger-Reissner (mixed) formulation where the symmetry of the stress tensor σ is dealt with in a weak form by introducing a Lagrange multiplier that represents the conservation of angular momentum. We consider the space of tensors whose rows consist of an element of RT_k space for the stress, the space of discontinuous piecewise linear vectors for the velocity, and the space of skew-symmetric continuous piecewise linear tensors to impose the symmetry weakly. We end up with a stress-velocity-vorticity formulation discretized with $RT_k^d - DP_k^d - P_k^{\frac{d(d-1)}{2}}$, where $k \geq 1$. This formulation has notable benefits, as it directly arises from the fundamental physical principles of momentum balance, constitutive law, and mass conservation. Moreover, it provides a direct presentation of stress, which is particularly crucial in certain applications. Numerical examples in both convex and non-convex two and three dimensional domains are presented to illustrate the efficiency of the proposed methodology.

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Stokes equation with non smooth boundary data

Katharina Lorenz[1] Thomas Apel[2] Johannes Pfefferer[3]

For the Dirichlet Boundary Control of the Stokes equation, it must first be discussed how to understand the solution of the Dirichlet problem for the Stokes equations when the Dirichlet data is not smooth, i.e. when it is only in $L^2(\Omega)$.

A weak solution $(y, p) \in H^1(\Omega)^2 \times L^2(\Omega)$ cannot be expected. Instead, the very weak formulation is considered and existence and uniqueness results are given. In addition, the regularity of the solution is discussed, when the boundary data is in $H^{\frac{1}{2}-s}(\Omega)$ with $s \in [0, 1]$. For the discretization, the regularization approach is considered and it is shown how to correctly handle the compatibility condition $\int u \cdot n = 0$. Discretization error estimates are presented and validated by numerical examples.

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Notes on session “Shape Optimisation (Küchwald 2-3)”

Constrained L^p Approximation of Shape Tensors and its Relation to Shape Gradients

Gerhard Starke[1] Laura Hetzel[2]

The recent pioneering work by Deckelnick, Herbert and Hinze [1] enables the approximation of the shape gradient with respect to $W^{1,\infty}$, the natural norm for the space of shape deformations in this context. An alternative route towards such shape gradients is investigated in [3] via the constrained L^p best approximation of shape tensors. The shape gradient appears as Lagrange multiplier in the corresponding optimality system. Shape tensors were introduced earlier, with a different motivation, by Laurain and Sturm in [2]. We review the main result from [3] on the relation between the above best approximation in L^p $(p \in (1,2])$ and the shape gradient in W^{1,p^*} $(1/p + 1/p^* = 1)$. Moreover, we generalize this result to the symmetric best approximation of shape tensors which is related to an elasticity-type norm. The numerical realization by lowest-order Raviart-Thomas elements for the shape tensor approximation is also presented and tested for several shape optimization problems of variable difficulty including state-of-the-art test problems.

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Continuation applied to Shape Optimization

Bernhard Endtmayer[1] Alessio Cesarano[2] Peter Gangl[3]

In this presentation, we propose a homotopy method for shape optimization. Newton's method provides quadratic convergence if the initial guess is close enough. However, a good initial guess is just available in rare cases. Here, we connect solution of a given we want to the solution to an "easier" problem. The idea is to follow this path until, we reach the desired solution. We follow the path using a predictor corrector algorithm. Finally, we use the predictor corrector method in shape optimization and provide a numerical example.

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Shape Optimization of the Thermoelastic Body Under Thermal Uncertainties

Viacheslav Karnaev[1] Helmut Harbrecht[2] Marc Dambrine[3] Giulio Gargantini[4]

We consider shape optimization problems in the framework of the thermoelasticity model under uncertainties on the input parameters in Robin's condition in the heat conduction equation. The purpose of considering this model is to account for thermal residual stresses or thermal deformations, which in case of high environmental temperature may hinder the mechanical properties of the final design. Then, the presence of uncertainty in the external temperature especially must be taken into account to ensure the correct manufacturing process and device performance. The presented theory applies to the minimization of the volume under constraints on the expectation of the the L^2-norm of the von Mises stress. We show that the robust constraints and its gradient are completely determined by low order moments of the random input. We derive a deterministic algorithm based on low-rank approximation and level-set method for the numerical solution and present model cases in shape optimization.

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Notes on session “Shape Optimisation (Küchwald 2-3)”

Space-time FEM for distributed optimal control problems subject to the wave equation with state or control constraints

Richard Löscher[1] Olaf Steinbach[2]

In this talk, we will briefly recall a unified abstract framework for the treatment of distributed optimal control problems subject to PDEs. Then, we will cast the optimal control problem subject to the wave equation with state constraints into this framework, using a space-time energy regularization. This approach will allow a full analysis of the problem at both the continuous and the discrete level.

In particular, we will provide regularization and finite element error estimates, from which we can derive an optimal relation between the regularization parameter and the mesh size, balancing accuracy and cost. Furthermore, we will demonstrate that the incorporation of control constraints into this framework requires only minor modifications.

The theoretical findings will be supported by numerical examples addressing both types of constraints.

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Dual-weighted residual goal-oriented error estimation for space-time adaptivity in phase-field fracture

Viktor Kosin[1] Amélie Fau[2] François Hild[3] Thomas Wick[4]

This presentation focuses on space-time adaptivity for phase-field fracture problems. The methodology requires a space-time formulation and utilizes a space-time Galerkin finite element discretization for the governing phase-field equations. Then, goal functionals (i.e., quantities of interest) are introduced. The computational implementation of goal-oriented error control employs the dual-weighted residual method in which an adjoint problem must be solved. As the analysis is quasi-static, without a temporal derivative, the adjoint problem of the quasi-static primal problem decouples in time. Nonetheless, time-averaged goal functionals can also be considered. The temporal and spatial errors are localized using a partition of unity, which allows one to adaptively refine and coarsen the time intervals and space elements in the space-time cylinder. Numerical tests are performed on a single edge notched tensile and shear test to investigate the quality of the proposed error estimator.

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A non-symmetric space-time coupling of finite and boundary element methods for a parabolic-elliptic interface problem

Günther Of[1] Tobias Kaltenbacher[2] Olaf Steinbach[3]

We consider the interface problem of the heat equation in a bounded domain and of the Laplace equation in the exterior domain. We present a coupling of a space-time formulation of the heat equation and the weakly singular integral equation of the Laplace equation and consider a conforming space-time discretization. We discuss an analysis of the proposed space-time formulation, an implementation of the related FEM-BEM coupling, and numerical tests.

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Notes on session “Space-Time (Küchwald 1)”

Frequency-Domain Formulation and Convergence Analysis of Biot’s Poroelasticity Equations Based on Total Pressure

Cristian Cárcamo[1] Alfonso Caiazzo[2] Felipe Galarce[3] Joaquín Mura[4]

In this talk, we discuss the well-posedness and error analysis of the Biot’s Poroelastic equations. To demonstrate the solvability of the poroelastic continuous issue, we first use the well-known Fredholm Alternative. In order to improve computational efficiency and address the issues raised by the discrete inf-sup condition, we present a novel and stable stabilized numerical system that is tuned for equal polynomial order. Additionally, we conduct a numerical analysis to determine the stability of solutions and provide an a priori error analysis. Finally, we present some numerical examples that offer strong evidence of the usefulness and effectiveness of the proposed numerical framework.

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Stress-based least-squares FEM for Elastoplasticity

Henrik Schneider[1]

For the discretization of the variational inequalities modelling elastoplastic material behaviour, a constrained first-order system least squares formulation is proposed and investigated. This approach allows the simultaneously finite element approximation of displacement and stresses, in the Sobolev spaces H^1 and $H(\mathrm{div})$, respectively. The coercivity of the underlying bilinear form is proved under suitable assumptions on the hardening laws for a plastic flow rule of von Mises type. Our formulation is momentum-conservative in an element-wise fashion and does not degenerate for (nearly) incompressible materials. This is even true if piecewise affine continuous functions (for the displacement components) are combined with lowest-order Raviart-Thomas elements (for the rows of the stress tensor). A semi-smooth Gauß-Newton method is set up based on the Newton derivative for the solution of the arising non-smooth nonlinear problems. Finally, computational results for common benchmark examples are shown including experiments for the limiting case of perfect plasticity.

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Notes on session “Solid Mechanics (Küchwald 4)”

A well-balanced finite element scheme based on monolithic convex limiting

Petr Knobloch[1] Dmitri Kuzmin[2] Abhinav Jha[3]

To obtain accurate approximate solutions, the used numerical scheme have to be consistent with the solved problem in an appropriate sense. One possible requirement is that the scheme preserves some simple solutions (equilibria) of the continuous problem, which is particularly important when inhomogeneous balance laws are considered. Discretizations that provide such consistency are called well balanced in the literature. We will consider this property in the context of finite element discretizations of steady convection-diffusion-reaction equations.

Recently, a well-balanced and positivity-preserving finite element scheme was developed by Hajduk (2022) for the inhomogeneous shallow water equations using the framework of algebraic flux correction. The monolithic convex limiting (MCL) algorithm presented in Hajduk (2022) and Hajduk, Kuzmin (2022) incorporates discretized bathymetry gradients into the numerical fluxes and intermediate states of the spatial semi-discretization. In the present contribution, we show that the source term of a scalar convection-diffusion-reaction problem can be treated similarly. In particular, we define numerical fluxes that ensure consistency of the well-balanced MCL approximation with a linear steady state. Using a convex decomposition into intermediate states, we enforce positivity preservation, as well as local and global discrete maximum principles. Moreover, the design of the method enables to prove that the nonlinear discrete problem possesses a solution. Numerical results illustrate potential benefits of well-balanced flux limiting in the scalar case. Details can be found in Knobloch, Kuzmin, Jha (2024).

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Properties of the Iterated penalty method for Scott-Vogelius elements

Franziska Eickmann[1] Ridgway Scott[2] Tabea Tscherpel[3]

Using the Scott-Vogelius mixed finite element spaces for solving the Stokes equations yields exactly divergence free velocity approximations. Therefore, the method is pressure-robust. The Scott-Vogelius velocity solution can be approximated by the iterated penalty method (IPM). This is an Uzawa-type iteration that does not require an explicit local basis of the pressure space.

We propose a local mesh modification that removes nearly singular vertices. By this we obtain convergence in few iterations and high accuracy in both the velocity and pressure approximation. It is well known that the velocity divergence converges to zero geometrically, but we also prove that it always decreases monotonically. Furthermore, we present a quasi-optimality estimate for the velocity approximation in each step of the IPM iteration which quantifies the influence of the pressure best approximation error. All of this can be done for inhomogeneous boundary conditions.

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Pressure-Robustness, an Elephant in the Room, and a Conceptual Review for Mixed Finite Element Methods

Alexander Linke[1] Christian Merdon[2] Nicolas Gauger[3]

In recent years, the notion of pressure-robustness aimed at overcoming an “elephant in the room” in the discretization theory of inf-sup stable mixed finite element methods for incompressible fluid dynamics. Originally coined “poor mass conservation”, the issue provoked some headache in theory and practice since the 1980ies, and has been traced back finally to an inappropriate discrete treatment of gradient fields, which lie in the kernel of a semi norm quantifying the strength of data driving the flow dynamics. Subsequently, pressure-robust flow discretizations have been constructed, which allow for error estimates that are qualitatitively different to the classical ones presented in the influential textbook by Girault and Raviart. Morevover, not only error estimates, but also basic concepts of mixed methods have been reviewed in the research on pressure-robustness, This concerns the notion of data, the appropriate conformity, the used model problems, and even the notion of locking, which is central for classical mixed finite element theory. Some history and various numerical examples illustrate the findings.

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Distributional finite elements for linearised Einstein–Bianchi equations

Edoardo Bonetti[1] Joachim Schöberl[2]

The Einsten-Bianchi (EB) equations are notoriously known in the relativity's community. The splitting of the Riemann tensor into a ”tidal” part and ”frame dragging” part carries, not only desired symmetries, but also a easy-to-understand physical meaning.

After deriving the linearized EB system, a novel normal-tangential distributional element is constructed and applied.

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Notes on session “Mixed Discretizations (Küchwald 2-3)”

Partition-of-unity localizations of dual-weighted residual estimators for single and multiple goal functionals

Thomas Wick[1] Thomas Richter[2] Bernhard Endtmayer[3] Ulrich Langer[4] Andreas Schafelner[5] Julian Roth[6] Jan Philipp Thiele[7]

In this talk, we present our efforts over the last years to apply partition-of-unity localizations in a posteriori goal-oriented error control and adaptivity for stationary and nonstationary problems. The partition-of-unity greatly facilitates error localization for nonlinear problems, coupled problems, multiphysics applications, up to space-time coupled variational inequality systems. We discuss the idea, concepts and show several applications in single and multigoal-oriented error estimation.

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Local isogeometric mesh refinement in polar-type domains with corners

Philipp Zilk[1] Thomas Apel[2]

Corner singularities play a significant role for the modeling of complex physical phenomena in non-smooth domains. Their presence renders simulations challenging as standard methods produce suboptimal results due to singular solutions. In isogeometric analysis, two-dimensional polar-type domains with corner singularities like circular sectors or L-shapes can be discretized conveniently with a single patch. However, the corresponding isogeometric parameterization is singular and standard approximation spaces are not appropriate.

Hence, two major challenges need to be tackled at once: the singularity of both the solution and the parameterization at the polar point. We introduce a graded mesh refinement algorithm, enabling locally refined meshes near the singular corner and combine it with modified approximation spaces that have been proposed for singularly parameterized domains in the literature. We prove optimal convergence of our method for solving boundary value and eigenvalue problems. To confirm the theory, we provide a series of numerical results.

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Adaptive mesh refinement for the Landau–Lifshitz–Gilbert equation

Stefan Karch[1] Jan Bohn[2] Willy Dörfler[3] Michael Feischl[4]

The Landau–Lifshitz–Gilbert (LLG) equation serves as a fundamental model for describing micromagnetic phenoma with applications in areas such as magnetic sensors, recording heads, and magneto-resistive storage devices. The applications have in common that they admit a strong locality in both time and space, e.g., sharp interfaces in domain walls. This characteristics encourages the utilization of adaptive methods.

To address these issues, we propose a novel time- and space adaptive algorithm for approximating the Landau–Lifshitz–Gilbert equation using a higher-order tangent plane scheme. Our approach relies on the linearly implicit backward difference formula (BDF) for time discretizations combined with standard higher order conforming finite elements and a Lagrangian setting to cope with the nonlinear constraint for the space discretization. The underlying methods have been developed and analysed in the uniform setting by Akrivis et al., (Higher-order linearly implicit full discretization of the Landau–Lifshitz–Gilbert equation, Math. Comput. 2021).

To derive our full adaptive integrator for LLG, we combine an estimate of the truncation error in time with the gradient recovery estimator for the spatial error. Moreover, we establish that under regularity assumptions, restrictions on the time step changes as well as on the damping term that the adaptive method satisfies a discrete energy estimate. Finally, we demonstrate in several numerical experiments the effectiveness of the proposed algorithm in comparison to uniform approaches.

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On full linear convergence and optimal complexity of adaptive FEM with inexact solver

Philipp Bringmann[1] Michael Feischl[2] Ani Miraçi[3] Dirk Praetorius[4] Julian Streitberger[5]

The ultimate goal of any numerical scheme for partial differential equations (PDEs) is to compute an approximation of user-prescribed accuracy at quasi-minimal computational time. To this end, the algorithmic realization of a standard adaptive finite element method (AFEM) integrates an inexact solver and nested iterations with discerning stopping criteria to balance the different error components. The analysis ensuring optimal convergence order of AFEM with respect to the overall computational cost critically hinges on the concept of R-linear convergence of a suitable quasi-error quantity. This talk presents recent advances in the analysis of AFEMs to overcome several shortcomings of previous approaches. First, a new proof strategy with a summability criterion for R-linear convergence allows to remove typical restrictions on the stopping parameters of the nested adaptive algorithm. Second, the usual assumption of a (quasi-)Pythagorean identity is replaced by the generalized notion of quasi-orthogonality from [Feischl, Math. Comp., 91 (2022)]. Importantly, this paves the way towards extending the analysis to general inf-sup stable problems beyond the energy minimization setting. Numerical experiments investigate the choice of the adaptivity and stopping parameters.

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Notes on session “Adaptivity (Küchwald 1)”

Modal analysis in mixed finite element methods

Önder Türk[1]

Modal analysis is a widely used approach to approximate solutions of time dependent problems of continuum mechanics. The equilibrium equations are transformed into an eigenvalue problem in which the eigenfunctions are the amplitudes and the eigenvalues are the squares of the frequencies. In the case of symmetric and positive definite operators such as elasticity, a complete set of eigenfunctions and associated positive eigenvalues exist, and therefore the true solution can be expressed as a series of modes. When mixed formulations are required as in the case of incompressible elasticity, and spatial discretisations based on the Galerkin variational form for the class of saddle-point problems are used, it is well known that the approximations are optimally convergent if the finite element spaces for different fields satisfy suitable inf-sup conditions. The stability issues when classical mixed methods are used with arbitrary interpolations violating this condition can be avoided by numerous stabilisation techniques. These apply to both the stationary boundary value problems and the associated eigenvalue problems. An extra care is needed when the latter is to be approximated by a residual based approach which may lead to a quadratic problem even if the original one is linear.

In this presentation we first describe a mixed finite element formulation for such eigenvalue problems that preserve the linearity of the continuous problem and can be solved using arbitrary interpolations for the unknown fields. The approach is mainly based on the variational multiscale concept which assumes that the unknown can be split into a finite element component and a subgrid scale to be modelled. The key point is to consider that this subgrid scale is orthogonal to the finite element space. Next, we present the extension of modal analysis for elastic materials and show that each pair (amplitude and frequency) can be obtained from an eigenvalue problem that can be split into the finite element scale and the subgrid scale. A set of solution pairs of this eigenvalue problem are computed, and finally the time approximation to the continuous solution is obtained taking a few modes, those associated with higher energy.

The presentation is based on joint work with D. Boffi from KAUST, Saudi Arabia, and R. Codina from UPC, Spain.

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On Embedded Trefftz discontinuous Galerkin methods

Igor Voulis[1] Philip L. Lederer[2] Christoph Lehrenfeld[3] Paul Stocker[4]

The central idea of Trefftz discontinuous Galerkin (DG) methods is to construct optimal discretization spaces that minimize the number of unknowns in a system while retaining optimal approximation properties. We discuss an approach aimed at reducing the system size in more general discontinuous Galerkin methods for partial differential equations (PDEs), drawing inspiration from Trefftz methods. Only the simplest (differential) operators operate suitably on discrete polynomial spaces. Other operators cause additional challenges. We discuss how to deal with these challenges, extending the scope in which the Trefftz DG method can be applied.

References:

[1] Lehrenfeld, C. & Stocker, P.: Embedded Trefftz discontinuous Galerkin methods, International Journal for Numerical Methods in Engineering, 2023

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Convergence of a Riemannian gradient method for the Gross–Pitaevskii energy functional in a rotating frame

Mahima Yadav[1] Patrick Henning[2]

This talk focuses on the numerical approximation of ground states of rotating Bose-Einstein condensates. This requires the minimization of the Gross-Pitaevskii energy functional on a Riemannian manifold. As an iterative solver for finding such minimizers we propose a generalized Riemannian gradient method with Sobolev gradients and an adaptively changing metric. We prove that the scheme reduces the energy in each iteration and we further explore its global and local convergence properties. In particular, the local convergence rates can be explicitly quantified in terms of spectral gaps involving $E''(u)$, where E is the energy functional and u a ground state. The theoretical findings are supported by numerical experiments.

References:

[1] https://arxiv.org/pdf/2406.03885

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Notes on session “Mixed Discretizations (Küchwald 2-3)”

A hybridizable mass-conserving stress-yielding method for incompressible flow

Jay Gopalakrishnan[1]

In computational fluid dynamics, the proper treatment of the incompressibility constraint on the fluid velocity is an age-old subject of discussion. A relatively recent twist in this topic, arising from a series of developments by multiple authors, is the treatment of the incompressibility constraint using the Sobolev space H(div), the space of vector fields whose components and divergence are square integrable. With this as a starting point, we proceed to discuss a natural Sobolev space for viscous fluid stresses to pair with H(div) velocities. Simple new matrix finite elements for viscous stresses are developed. They have shear continuity and can be seen as arising from a nonstandard Sobolev space H(curl div). The resulting method, called the Mass-Conserving Stress-yielding (MCS) method, produces optimal order approximations for viscous stresses, velocity, pressure, and vorticity, is exactly mass conserving, and is pressure robust. Moreover, the method uses only facet-based coupling (i.e., without any vertex or edge degrees of freedom in three dimensions) and is amenable to straightforward hybridization. This is joint work with Philip Lederer and Joachim Schöberl.

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Discrete weak duality of hybrid high-order methods for convex minimization problems

Tran Ngoc Tien[1]

This talk derives a discrete dual problem for a prototypical hybrid high-order method for convex minimization problems. The discrete primal and dual problem satisfy a weak convex duality that leads to a priori error estimates with convergence rates under additional smoothness assumptions. This duality holds for general polyhedral meshes and arbitrary polynomial degrees of the discretization.

References:

[1] https://arxiv.org/abs/2308.03223

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Obtaining reliable simulations of industrial fluid flow applications

Ridgway Scott[1]

A new era in flight is emerging that requires a more effective simulation strategy. Many modes of transportation are being developed industrially, including air-taxi drones and ground-effect transport. Similarly, new modes of energy generation, such as blade-less wind farms have been proposed. All of these require a new level of reliability for simulations to be useful in engineering design. We will describe some computations we are doing and the flaws in standard algorithms that have been uncovered in the process. We will also describe some open problems related to these and some prizes being offered for their solution.

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[1] L. Ridgway Scott and Rebecca Durst. Chaotic dynamics of two-dimensional flows around a cylinder. Physics of Fluids 36, 024118 (2024), published online 16 Feb 2024.

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Notes on session “Fluid Flow (Küchwald 2-3)”

Weak maximum principle of finite element methods for parabolic equations

Dmitriy Leykekhman[1] Buyang Li[2]

Maximum principle is a fundamental mathematical tool to study elliptic and parabolic partial differential equations. The discrete counterpart of maximum principle associated to finite element methods has a long history of research and remains an active field. Unlike its continuous counterpart, the discrete maximum principle is not an inherent property and is significantly influenced by the triangulation of the physical domain. In dimensions three and higher, it becomes challenging to assure the discrete maximum principle for even piecewise linear elements. Nonetheless, a large number of applications do not require a strong discrete maximum principle. In 1980, A. Schatz demonstrated that a weak maximum principle (also known as the Agmon-Miranda principle) is applicable to a broad spectrum of finite elements on general quasi-uniform triangulation in any two-dimensional polygonal domains, which was later extended to three dimensions. The situation for parabolic equations is more complex, depending not only on space discretization but also on time discretization. In my talk I will review the history of the weakened strong discrete maximum principle and show new results that establish the weak maximum principle of finite element methods for parabolic equations semidiscrete and fully discrete Galerkin finite element solutions.

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Adaptive parallel space-time discontinuous Galerkin Methods for the linear transport equation

Christian Wieners[1]

We consider variational space-time discretizations for the linear transport equation with full upwind discontinuous Galerkin methods in space and time. Based on our convergence analysis for symmetric Friedrichs systems in a mesh-dependent DG norm we construct an error indicator and show numerically that the adaptive method is efficient. The linear system is solved by a multigrid method in space and time, and we show numerically that the convergence is of optimal complexity. We observe that convergence is obtained also in case of discontinuous solutions without regularity requirements. Then we show that in case of local sources and local goal functionals the computational domain can be restricted to a subset of the space-time cylinder and that then a suitable parallel strategy results in a significant reduction of the computational effect. Finally, the discretization is compared with the analysis of an overlapping DGP method which provides convergence estimates with minimal regularity requirements.

References:

[1] https://doi.org/10.1016/j.camwa.2023.10.031

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Space-time least-squares finite element methods

Christian Köthe[1] Richard Löscher[2] Olaf Steinbach[3]

For the numerical solution of an operator equation $Bu = f$ we consider a least-squares approach. We assume that $B : X \to Y^*$ is an isomorphism and that $A : Y \to Y^*$ implies a norm, where X and Y are Hilbert spaces.

Firstly, we assume the differential operator B to be linear. The minimizer of the least-squares functional $\frac{1}{2} \|Bu - f\|_{A^{-1}}$ is then characterized by the gradient equation which involves an elliptic operator $S = B^* A^{-1} B : X \to X^*$. We introduce the adjoint $p = A^{-1}(f - Bu)$ and reformulate the first order optimality system as a saddle point system. Based on a discrete inf-sup condition we discuss related a priori error estimates and use the discrete adjoint p_h to drive an adaptive refinement scheme. Numerical examples will be presented which confirm our theoretical findings. Secondly, we demonstrate how to apply the least-squares approach for the numerical solution of a non linear operator equation $B(u) = f$. We derive the related first order optimality system and discuss its solution via Newton's method. Numerical examples involving the semi-linear heat equation and the quasi-linear Poisson equation will be presented.

Finally, we will conclude with some remarks on future work in this area which needs to be done.

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[1] C. Köthe, R. Löscher, O. Steinbach: Adaptive least-squares space-time finite element methods. arXiv:2309.14300, 2023.

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A priori error estimates for finite element discretization of semilinear elliptic equations with non-Lipschitz nonlinearities

Boris Vexler[1]

In this talk we discuss the finite element discretization of semilinear elliptic equations with nonlinearities, which are only assumed to be monotonically non-decreasing and continuous. This means, that non-differential, non-Lipschitz and even non-Hölder continuous nonlinearities are allowed. For a large class of such equations (posed on a polygonal/polyhedral and convex domain) we provide a priori error estimates for a direct finite element discretization (without any regularization).

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Notes on session “Space-Time (Küchwald 2-3)”

Higher order temporal derivarives of the initial conditions for time-dependent generalized Stokes problems

Gunar Matthies[1]

We consider the two-parametric family of variational time discretizations that generalizes the well-known discontinuous Galerkin (dG) and continuous Galerkin-Petrov (cGP) methods. This family of time discretizations allows for higher order schemes with higher order regularity, provided that sufficiently accurate approximations of the higher order derivatives of the solution at initial time are known.

We will discuss how these accurate approximations can be obtained for generalized time-dependent Stokes problems. Two different scenarios will be considered. We start with standard inf-sup stable finite element discretizations in space and show optimal error bounds for the higher order time derivatives of both velocity and pressure at initial time. The second setting deals with pressure-robust inf-sup stable spatial discretizations. We use a reconstruction operator to ensure pressure robustness. For this case, we prove optimal error estimates for higher order time derivatives of velocity at initial time that are completely independent of pressure.

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Towards dissipative solutions of turbulent incompressible flows

Gert Lube[1]

$H(\text{div})$-conforming DG methods can be used to generate point-wise divergence-free velocities for incompressible flow problems. Such methods can be shown to be pressure-robust and convection-semi-robust. It is a challenge to show that they generate dissipative solutions for turbulent flows in the Euler limit case. We discuss some difficulties of such approach.

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Trefftz-DG discretization for the Stokes problem

Paul Stocker[1] Philip L. Lederer[2] Christoph Lehrenfeld[3]

We introduce a new discretization based on a polynomial Trefftz-DG method for solving the Stokes equations. Discrete solutions of this method fulfill the Stokes equations pointwise within each element and yield element-wise divergence-free solutions. Compared to standard DG methods, a strong reduction of the degrees of freedom is achieved, especially for higher polynomial degrees. In addition, in contrast to many other Trefftz-DG methods, our approach allows us to easily incorporate inhomogeneous right-hand sides (driving forces) by using the concept of the embedded Trefftz-DG method. We present a detailed a priori error analysis and numerical examples.

References:

[1] https://doi.org/10.1007/s00211-024-01404-z

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Augmenting the grad-div stabilization for Taylor-Hood finite elements with a vorticity stabilization

Marwa Zainelabdeen[1]

The least squares vorticity stabilization (LSVS), proposed in [2] for the ScottVogelius finite element discretization of the Oseen equations, is studied as an augmentation of the popular grad-div stabilized Taylor-Hood pair of spaces. An error analysis is presented which exploits the situation that the velocity spaces of Scott-Vogelius and Taylor–Hood are identical. Convection-robust error bounds are derived under the assumption that the Scott-Vogelius discretization is well posed on the considered grid. Numerical studies support the analytic results and they show that the LSVS-grad-div method might lead to notable error reductions compared with the standard grad-div method.

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Notes on session “Fluid Flow (Küchwald 1)”

Sparse source detection for advection-diffusion problems

Marco Mattuschka[1] Max von Danwitz[2] Alexander Popp[3]

This talk presents an application of sparse optimization techniques for advection-diffusion problems. The advection-diffusion equation is suitable for describing the dispersion of a pollutant concentration $u : (0, T) \times \Omega \to \mathbb{R}$:

$$\begin{aligned} u_t - \kappa \Delta u + \mathbf{v} \cdot \nabla u &= 0 && \text{in } (0,T) \times \Omega, \\ \kappa \nabla u \cdot \eta &= 0 && \text{in } (0,T) \times \Gamma_N, \\ u &= 0 && \text{in } (0,T) \times \Gamma_D, \\ u(0, \cdot) &= m && \text{in } \Omega. \end{aligned}$$

While the forward problem $\mathcal{F}(m) = u$ describes the evolution of u over time, the aim of the inverse problem is to predict the source of the pollutant based on several discrete noisy sensor measurements d. Since the release of pollutants under real conditions is very localized, an approach was chosen that promotes sparsity in m. To model this, an optimization problem is formulated for the initial value m

$$\min_{m \in \mathcal{M}} \frac{1}{2} ||\mathcal{F}(m) - d||^2_{\Gamma^{-1}_{\text{noise}}} + \alpha \, \|m\|_{\mathcal{M}(\Omega)} \, .$$

The regularization requires, that m is in the space of regular Borel measures $\mathcal{M}(\Omega)$ understood as a dual space of the continuous functions $C(\Omega)$:

$$\|m\|_{\mathcal{M}(\Omega)} = \sup\{\langle m, \varphi \rangle : \varphi \in C(\overline{\Omega}), \|\varphi\|_{C(\overline{\Omega})} = 1\}.$$

For the numerical solution, the linear advection-diffusion equation and the corresponding adjoint equation is discretized by standard stabilized continuous Galerkin FEM methods. For the solution of the inverse problem a Primal-Dual-Active-Point strategy (PDAP) is used. The talk is mainly intended to discuss the near real-time capabilities of this method and its applicability for the protection of critical infrastructures (KRITIS).

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[1] https://doi.org/10.1051/cocv/2021042

[2] https://iopscience.iop.org/article/10.1088/1361-6420/ad2cf8

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Solving Nonlinear Virus Replication PDE Models With Hierarchical Grid Distribution Based GMG

Markus M. Knodel[1] Arne Nägel[2] Eva Herrmann[3] Gabriel Wittum[4]

Realistic biophysical models in general only can be evaluated by applying advanced numerical solution techniques. The recent COVID19 pandemics has unveiled the need for detailed biophysical understanding of virus replication mechanisms. We are building a framework to mirror intracellular virus replication dynamics by means of fully spatio-temporal resolved PDE models. The models couple effects which are restricted to intracellular 3D embedded 2D curved manifolds with the full 3D intracellular space dynamics. Technically, surface PDEs (sufPDE) are coupled with PDE by the aid of boundary conditions for the PDEs which are reflected by reaction terms of the sufPDEs. The highly nonlinear sufPDE/PDE system is discretized with vertex centered Finite Volumes (vcFV) upon unstructured grids which are reconstructed from experimental data. This study describes the properties of the application of a hierarchical grid distribution based Geometric Multigrid Solver (GMG) to the system of linear equations (SLE) established by a nonlinear Newton solver. We demonstrate the precision and efficient weak scaling up to about 300 Millions degrees of freedom (DoFs) at grid refinement level 4 based on the massively parallel GMG solver implemented in UG4. The biophysical output data demonstrate quantitative consistence with the experimental findings, prompting further advanced experimental studies to validate the model and refine our quantitative biophysical understanding. Our framework allows for realistic intracellular virus replication simulations paving new ways for the development of direct antiviral agents and potent vaccines.

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Theoretical aspects of the finite element method in solving fractional wave equations with nonsmooth data

Reza Mokhtari[1] Mohadeseh Ramezani[2] Yubin Yan[3]

We aim to focus on the finite element method (FEM) based on a corrected formula designed for solving the following fractional wave equation

$$\begin{cases} {}_0^C\mathrm{D}_t^\alpha u + \mathcal{L}u = f(t), & 0 \le t \le T, \\ u(0) = u_0, & u'(0) = u_1, \end{cases}$$

where ${}_0^C\mathrm{D}_t^\alpha$ is the Caputo fractional derivative with respect to t, i.e.

$${}_0^C\mathrm{D}_t^\alpha u(t) = \frac{1}{\Gamma(2-\alpha)} \int_0^t (t-s)^{1-\alpha}\, u''(s)\,\mathrm{d}s, \qquad \alpha \in (1,2),$$

in which $\Omega \subset \mathbb{R}^d$, $d = 1,2,3$, $\mathcal{L} = -\Delta$ that is the Laplacian with the definition domain $D(\mathcal{L}) = H_0^1(\Omega) \cap H^2(\Omega)$, and $u_0, u_1 \in L^2(\Omega)$ are some given functions. This model problem has applications in modeling processes characterized by non-local effects such as anomalous diffusion and infiltration. It highlights the importance of maintaining temporal accuracy when dealing with nonsmooth data. Traditional numerical schemes often struggle to maintain the desired temporal order of convergence in such scenarios. The complexities of fractional wave equations, especially when nonsmooth initial or source data are involved, worsen these challenges, leading to a breakdown in the accuracy and efficiency of classic methods. Our approach introduces a corrected scheme within the FEM framework that is specifically designed to preserve temporal order, even in the presence of nonsmooth data. Leveraging time discretization techniques with an enhanced correcting initial step, our method overcomes the limitations of conventional approaches. The theoretical foundation of this method is grounded in the Laplace transform method. We present analysis of the method's performance, including error estimates. Finally, we confirm the theoretical results using a numerical example.

References:

[1] M. Ramezani, R. Mokhtari, Y. Yan, Correction of a high-order numerical method for approximating time-fractional wave equation. Journal of Scientific Computing, 100(3), 71, (2024).

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Preconditioning for a phase-field model for the morphology evolution in organic solar cells

Pelin Çiloğlu[1] Roland Herzog[2] Jan-Frederik Pietschmann[3] Martin Stoll[4] Carmen Tretmans[5]

In this study, we address the numerical investigation of a phase-field model for the formation of acceptor and donor regions during the production of organic solar cells. This process is driven by the spinodal decomposition of two species in a solvent, where the solvent evaporates, resulting in a coupling of phase field equations via degenerate mobility. The model, described by coupling the Cahn–Hilliard equations and Navier-Stokes equations, is discretized using a finite element approach. To solve the resulting large-scale linear systems efficiently, we introduce a preconditioning strategy based on efficient approximations of the Schur-complement of a saddle point system. To illustrate the efficiency of our methodology, we provide several numerical examples.

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Notes on session “Solvers (Küchwald 4)”

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