Austrian Numerical Analysis Day

and Colloquium dedicated to Ulrich Langer and Walter Zulehner on the occasion of their retirement

4 – 6 May 2022, RICAM & JKU, Linz

Wednesday, 4 May 2022

12:30 − 13:45	Registration		
13:45 − 14:00	Opening		
14:00 − 15:30	**Colloquium session**		Chair: Herbert Egger
14:00 − 14:30	Heinz Engl	From Hans-Jörg Wacker via Walter Zulehner to Ulrich Langer: personal recollections about a very successful time for applied mathematics in Linz	
14:30 − 15:00	Dietrich Braess	Approximation of $1/\|x\|^\alpha$ by exponential sums and multidimensional integrals: From Heron to multidimensional integrals	
15:00 − 15:30	Joachim Schöberl	NGSolve – a finite element package for teaching and research	
15:30 − 16:00	Coffee Break		
16:00 − 17:30	**Colloquium session**		Chair: Clemens Hofreither
16:00 − 16:30	Dirk Pauly	Hilbert Complexes and PDEs	
16:30 − 17:00	Jarle Sogn	Operator precondition for multiple saddle point problems	
17:00 − 17:30	Stefan Takacs	Domain Decomposition Methods for the Stokes and elasticity problems in Isogeometric Analysis	

Thursday, 5 May 2022 – Morning

8:30 – 9:00	Registration	
9:00 – 10:30	**Colloquium session**	Chair: Günther Of
9:00 – 9:30	Wolfgang L. Wendland	Boundary Integral Equations for Scattering by a Perfect Electric Conductor
9:30 – 10:00	Wolfgang Hackbusch	Computation of Optimal Exponential Sums w.r.t. the Maximum Norm
10:00 – 10:30	Gabriel Wittum	Double enriched finite volume spaces for the DNS of fluid-particle interaction
10:30 – 11:00	Coffee Break	
11:00 – 12:30	**Colloquium session**	Chair: Stefan Takacs
11:00 – 11:30	Clemens Hofreither	(Best) Rational Approximation and Fractional Diffusion
11:30 – 12:00	Gundolf Haase	CFD Simulations in Cardivascular Systems
12:00 – 12:30	Olaf Steinbach	Space-time finite and boundary element methods
12:30 – 14:00	Lunch	

Thursday, 5 May 2022 – Afternoon

13:00 − 14:00	Registration	
14:00 − 16:05	**ANADay session**	Chair: Olaf Steinbach
14:00 − 14:25	Julia I.M. Hauser	A Space-Time Finite Element Method for the vectorial wave equation under consideration of Ohm's Law
14:25 − 14:50	Marco Zank	Direct Space-Time Solvers for a Conforming FEM for the Wave Equation
14:50 − 15:15	Alessio Cesarano	Space-time optimization of rotating electric machines
15:15 − 15:40	Mario Gobrial	Space-Time Finite Element Methods in Moving Domains
15:40 − 16:05	Richard Löscher	Towards unconditionally stable space-time FEM for the wave equation
16:05 − 16:30	Coffee Break	
16:30 − 18:35	**ANADay session**	Chair: Ilaria Perugia
16:30 − 16:55	Martin Halla	Finite Element Approximation of Holomorphic Eigenvalue Problems
16:55 − 17:20	Othmar Koch	Adaptive Magnus-type integrators for the simulation of solar cells
17:20 − 17:45	Ani Miraçi	A-posteriori-steered and *hp*-robust multigrid solvers
17:45 − 18:10	Michael Neunteufel	Analysis of intrinsic curvature approximations with Regge finite elements
18:10 − 18:35	Nepomuk Krenn	Finite element analysis for topological derivatives of optimization problems subject to a linear PDE constraint
19:30 −	Conference Dinner	

Friday, 6 May 2022

9:00 – 10:40	**ANADay session**	Chair: Gundolf Haase
9:00 – 9:25	Peter Gangl	Application of topological derivative in discrete material optimiazton
9:25 – 9:50	Richard Kowar	Analysis for Full Field Photoacoustic Tomography with Variable Sound Speed
9:50 – 10:15	Ceyhun Özdemir	A 3D finite element - boundary element coupling method in time domain for the scalar wave equation
10:15 – 10:40	Raphael Watschinger	A Time-Adaptive Fast Multipole Boundary Element Method for the Heat Equation
10:40 – 11:10	Coffee Break	
11:10 – 12:50	**ANADay session**	Chair: Andreas Schröder
11:10 – 11:35	Maximilian Brunner	Rate-optimal goal-oriented adaptive FEM for semilinear elliptic PDEs
11:35 – 12:00	Christoph Augustin	An accurate and efficient finite element framework with applications to cardiac electromechanics
12:00 – 12:25	Douglas R. Q. Pacheco	Initial higher-order pressure convergence in unbalanced finite element discretizations of incompressible flow problems
12:25 – 12:50	Alexander Labovsky	Large Eddy Simulation with Correction (LES-C) – a new class of turbulence models

Approximation of $1/\|x\|^\alpha$ by exponential sums and multidimensional integrals: From Heron to multidimensional integrals

Dietrich Braess[1]

[1] University Bochum

Multidimensional integrals with Greens functions are decomposed into products of one-dimensional integrals if the function $1/\|x\|$ is approximated on $[1, \infty)$ by sums of exponentials. Here the asymptotics of the approximation order with $exp(-c\sqrt{k})$ can be determined by using results on rational approximation. The latter, in turn, are determined via Gauss' arithmetic-geometric mean. The method yields sharp estimates for the approximation on finite intervals. The results for the infinite interval provide the correct asymptotic behavior.

This presentation is scheduled for Wednesday, 4 May 2022, 14:30.

NGSolve – a finite element package for teaching and research

Joachim Schöberl[1]

[1] TU Vienna

In this talk we present the open source finite element library Netgen/NGSolve. We show how we can use its flexible Python front-end within jupyter-notebooks in class, and give some examples on recent research on matrix-valued finite elements in fluid dynamics, structural mechanics and numerical relativity.

This presentation is scheduled for Wednesday, 4 May 2022, 15:00.

Hilbert Complexes and PDEs

Dirk Pauly[1]

[1] TU Dresden, Germany

We discuss some aspects of Hilbert complexes and related PDEs.

This presentation is scheduled for Wednesday, 4 May 2022, 16:00.

Operator precondition for multiple saddle point problems

Jarle Sogn[1]

[1] University of Oslo, Norway

In this talk we consider multiple saddle point problems with block tridiagonal Hessian in a Hilbert space setting. We give a characterization of all block structured (nonstandard) norms, which ensure well-posedness and we relate this to the well-known Ladyzhenskaya–Babuška–Brezzi (LBB) conditions. This theory is a helpful tool for constructing block diagonal preconditioners for discretized problems, which we demonstrate on a Biot's consolidation model and on a general class of PDE-constrained optimal control problems.

This presentation is scheduled for Wednesday, 4 May 2022, 16:30.

Domain Decomposition Methods for the Stokes and elasticity problems in Isogeometric Analysis

Jarle Sogn[1] and Stefan Takacs[2]

[1] University of Oslo, Norway
[2] Johannes Kepler University Linz

We consider the discretization of the Stokes and elasticity equations using multi-patch Isogeometric Analysis. Both problems are formulated as a mixed system, which has saddle point structure. Well-posedness of the (discretized) system is usually shown by means of Brezzi's theorem. Besides the conditions that carry over from the (well studied) continuous case, there is one condition that has to be verified separately for the discretized problem: the inf-sup condition. For discretizations with single-patch Isogeometric Analysis, the inf-sup condition has already been shown for several discretizations. In the talk, we will see how inf-sup results for the single-patch case can be carried over to the multi-patch case. We will rediscover that the inf-sup constant heavily depends on the global geometry. For the elasticity equations, additional challenges arise from the Korn inequality. The efficient solution of the problem by means of a domain decomposition method, namely the Isogeometric Tearing and Interconnecting method, will be adressed. We will be very careful to avoid any dependence of the convergence behavior on the global inf-sup constant and the constant from the global Korn inequality. The presented theory and the numerical experiments confirm that we succeeded with this attempt.

This presentation is scheduled for Wednesday, 4 May 2022, 17:00.

Boundary Integral Equations for Scattering by a Perfect Electric Conductor

Wolfgang L. Wendland[1] and George C. Hsiao[2]

[1] Universität Stuttgart, Germany
[2] University of Delaware, USA

We consider the electromagnetic scattering problem in the exterior domain $\Omega_c = \mathbb{R}^3 \setminus \overline{\Omega}$ with constant elastic permittivity $\varepsilon > 0$ and magnetic permeability $\mu > 0$ around a perfect conductor Ω, a bounded Lipschitz domain in $\mathbb{R}^3$. In order to determine the time harmonic total fields with known frequency and given incident waves E^i, H^i, the Maxwell equations in the exterior domain for the scattered field E^s, H^s can be determined by solving electric field boundary integral equations EFIE on the boundary $\Gamma = \partial\Omega$ with boundary element methods. We are revisiting the basic works "Boundary element methods for Maxwell equations on non–smooth domains" by A. Buffa, M. Costabel and C. Schwab in Numer. Math. **92** (2002) 679–710 and "Boundary element methods for Maxwell transmission problems in Lipschitz domains" by A. Buffa, R.H. Hiptmair, T. von Petersdorff, C. Schwab in Numer. Math.**95** (2003) 459–485.

The EFIE form a strongly elliptic system of boundary integral equations whose numerical solution with Galerkin's boundary element method is asymptotically convergent with optimal order.

This presentation is scheduled for Thursday, 5 May 2022, 9:00.

Computation of Optimal Exponential Sums w.r.t. the Maximum Norm

Wolfgang Hackbusch[1]

[1] University Kiel, Germany

The approximation of the function $1/x$ by exponential sums has several interesting applications. It is well known that best approximations with respect to the maximum norm exist. Moreover, the error estimates exhibit exponential decay as the number of terms increases. Here we focus on the computation of the best approximations. In principle, the problem can be solved by the Remez algorithm, however, because of the very sensitive behaviour of the problem the standard approach fails for a larger number of terms. We present a stable algorithm.

This presentation is scheduled for Thursday, 5 May 2022, 9:30.

Double enriched finite volume spaces for the DNS of fluid-particle interaction

Jonas Simon[1], Susanne Höllbacher[2], and Gabriel Wittum[2]

[1] G-CSC, Goethe University Frankfurt, Germany
[2] CEMSE, KAUST, Saudi Arabia

We present double enriched finite volume spaces for the simulation of free particles in a fluid. This involves forces beeing exchanged between the particles and the fluid at the interface. In an earlier work we derived a monotithic scheme which includes the interaction forces into the Navier-Stokes equations by direct coupling. In multiphase flows oscillations and spurious velocities are a common issue. The surface force term yields a jump in the pressure and therefore the oscillations are usually resolved by extending the spaces on cut elements in order to resolve the discontinuity. For the construction of the enriched spaces proposed in this paper we exploit the Petrov-Galerkin formulation of the vertex-centered finite volume method (PG-FVM). From the perspective of the finite volume scheme we argue that wrong discrete normal directions at the interface are the origin of the oscillations. The new perspective of normal vectors suggests to look at gradients rather than values of the enriching shape functions. The crucial parameter of the enrichement functions therefore is the gradient of the shape functions and especially the one of the test space. The distinguishing feature of our construction therefore is an enrichment that is based on the choice of shape functions with consistent gradients. These derivations finally yield a fitted scheme for the immersed interface. We further propose a strategy ensuring a well-conditioned system independent of the location of the interface. Numerical tests were conducted using the PG-FVM. We demonstrate that the enriched spaces are able to eliminate the oscillations.

This presentation is scheduled for Thursday, 5 May 2022, 10:00.

(Best) Rational Approximation and Fractional Diffusion

Clemens Hofreither[1]

[1] Johann Radon Institute for Computational and Applied Mathematics (RICAM)

The numerical solution of fractional diffusion equations can under certain assumptions be viewed as the computation of a fractional power of a large, sparse matrix. We discuss how methods of rational approximation can be used to construct fast numerical solvers for such problems: in fact, many disparate numerical approaches can be cast into a unified rational approximation framework. In addition to direct rational approximation methods based on partial fraction decomposition, we also consider rational Krylov methods based on well-chosen poles for both elliptic and time-dependent fractional problems.

In many approaches, using the best uniform rational approximation to a function of the type $x^{-\alpha}$ leads to the best-in-class numerical methods. This leads naturally to the question of how to rapidly and accurately compute best rational approximations. We discuss recently developed algorithms such as BRASIL and a Newton's method for best uniform rational approximation, both of which make use of the so-called barycentric rational formula.

This presentation is scheduled for Thursday, 5 May 2022, 11:00.

CFD Simulations in Cardivascular Systems

Elias Karabelas[2,3,1], Jana Fuchsberger[1], Gundolf Haase[1], Federica Caforio[2,1], Steven Niederer[3], and Gernot Plank[2]

[1] University of Graz
[2] Medical University of Graz
[3] King's College London, United Kingdom

Simulating the total heart function includes CFD blood flow models which serve as the hydrodynamic load imposed on cardiac mechanics. Heart valves play a pivotal role in filling and ejection of cardiac chambers such as the left ventricle (LV). Thus, their functional representation in CFD simulations of hemodynamics in the LV and the attached aorta is vital. Usually this task is achieved using fluid-structure-interaction (FSI) where valves are modeled as thin structures.

We investigate the suitability of an alternative approach: A fictitious domain method is realized by extending the Navier-Stokes equation with a linear permeability term, which results in the Navier-Stokes-Brinkman equation. In this setting the permeability parameter is used to model a valve as a fictitious solid domain. The (fast) opening and closing of the valve is realized by changing the permeability within the finite elements which are covered by the moving valve in its current configuration. The underlying mesh representing the blood pool remains unchanged but the equations contain a volume fraction parameter denoting the degree of partial coverage of finite elements in the blood pool by the valve. To deal with turbulence occurring at higher Reynolds numbers the residual based variational multiscale (RBVMS) turbulence model [5, 6] was em- ployed. The RBVMS formulation has the additional property of stabilizing our method, which allowed the use of lowest equal order finite elements reducing also the implementation work in the cardiac modeling framework CARPentry. In this talk we will present ongoing validation work [4, 2] and applications stemming from clinical datasets [3, 1].

References

[1] J. Fuchsberger, P. Aigner, G. Haase, S. Niederer, H. Schima, G. Plank, E. Karabelas: "On the Incorporation of Obstacles in a Fluid Flow Prob- lem Using a Navier-Stokes-Brinkman Penalization Approach", Journal of Computational Science, 57 (2022); doi: 10.1016/j.jocs.2021.101506; arXiv:2009.03113.

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[3] J. Fuchsberger, E. Karabelas, P. Aigner, H. Schirma, G. Haase and G. Plank: "Validation study of computational fluid dynamics models of hemodynamics in the human aorta", in J. Proceedings in Applied Mathematics and Mechanics, 19(1), pp. e201900472 (2019-09-04), doi: 10.1002/pamm.201900472, No 72

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[6] Y. Bazilevs, K. Takizawa and T. E. Tezduyar: Challenges and directions in computational fluid-structure interaction: Methods and Applications, John Wiley & Sons, Hoboken, (2013)

This presentation is scheduled for Thursday, 5 May 2022, 11:30.

Space-time finite and boundary element methods

Olaf Steinbach[1]

[1] TU Graz

In this talk we will review some recent results on the stability and error analysis of space-time finite and boundary element methods. In addition to standard Bochner space formulations we also consider the variational formulation in anisotropic Sobolev spaces, where we use a modified Hilbert transformation to end up with a Galerkin-Bubnov method. Applications also include distributed optimal control problems subject to time-dependent partial differential equations.

This presentation is scheduled for Thursday, 5 May 2022, 12:00.

A Space-Time Finite Element Method for the vectorial wave equation under consideration of Ohm's Law

Julia I.M. Hauser[1]

[1] TU Dresden

In electromagnetism we can use the vectorial wave equation to describe problems. The equation arises from Maxwell's equations. Let us consider the vectorial wave equation in a 2D+1D space-time setting and treat time as another dimension. Hence we do not simplify the equation, but use partial integration in time and space for the variational formulation. Then we know that the resulting variational formulations for the vectorial wave equation is uniquely solvable. If we additionally apply Ohm's Law to the electromagnetic problem, linear dependencies arise in the right hand side. For this kind of equation we can still formulate uniquely solvable space-time variational formulations.
In this talk we will take a look at the numerical challenges of this problem. In addition to a CFL condition, we will see other challenges as well. We take a look at what kind of finite elements we have to choose to incorporate the whole problem and how the meshing effects our results. In the end we will discuss these numerical results of the vectorial wave equation.

This presentation is scheduled for Thursday, 5 May 2022, 14:00.

Direct Space-Time Solvers for a Conforming FEM for the Wave Equation

Marco Zank

Universität Wien

For the discretisation of time-dependent partial differential equations, the standard approaches are explicit or implicit time stepping schemes together with finite element methods in space. An alternative approach is the usage of space-time methods, where the space-time domain is discretised and the resulting global linear system is solved at once. In this talk, the scalar wave equation in second-order formulation serves as a model problem. First, a space-time variational setting is introduced, where a modified Hilbert transform is used such that ansatz and test spaces are equal. A conforming discretisation of this space-time variational formulation yields a space-time Galerkin finite element method, which is unconditionally stable, i.e., no CFL condition is required. However, this space-time Galerkin finite element discretisation leads to a large global linear system of algebraic equations. The main part of this talk investigates new efficient direct solvers for this system. In particular, a tensor-product approach with piecewise polynomial, globally continuous ansatz and test functions is used. The developed solvers are based on the Bartels–Stewart method and on the Fast Diagonalization method, which result in solving a sequence of spatial subproblems. The solver based on the Fast Diagonalization method allows solving these spatial subproblems in parallel, leading to a full parallelization in time. In the last part of the talk, numerical examples are shown and discussed.

This presentation is scheduled for Thursday, 5 May 2022, 14:25.

Space-time optimization of rotating electric machines

Alessio Cesarano[1], Charles Dapogny[2], Peter Gangl[1]

[1] Johann Radon Institute of Computational and Applied Mathematics (RICAM), Linz
[2] Laboratoire Jean Kuntzmann, Grenoble

Electric machines can often be modeled by the magneto-quasi-static approximation of Maxwell's equations in two space dimensions. We consider the simulation of a rotating electric machine by means of a space-time finite element method where the rotation is captured by the tetrahedral space-time mesh. We derive the shape derivative for a given cost function with respect to a perturbation of the (spatial) geometry and present a shape optimization algorithm for moving domains in space-time. Here, it is important to note that the optimized geometry is moving, but must not change its shape over time. To better explain our method and the related concepts, we first deal with an academic unconstrained optimization problem and show four scenarios one could consider, then we apply it to the time-dependent model of a rotating electric machine.

This presentation is scheduled for Thursday, 5 May 2022, 14:50.

Space-Time Finite Element Methods in Moving Domains

Mario Gobrial[1]

[1] TU Graz

Space-time discretization methods are well suited to handle moving domains in electric machines such as the electric motor. The space-time domain is discretized at once, and in contrast to time stepping methods the movement can be captured by a fixed space-time mesh. For the solution of the magento quasi-static Maxwell equations in the electric motor we formulate space-time finite element methods, considering a two-dimensional spatial domain and the time as the third dimension of the domain. As in the case of a fixed domain we are able to prove an inf-sup stability condition to ensure unique solvability. These space-time finite element methods allow for a parallel iterative computation for the magnetic flux density. Accordingly, the torque and the iron losses can be computed for the electric motor.

This presentation is scheduled for Thursday, 5 May 2022, 15:15.

Towards unconditionally stable space-time FEM for the wave equation

Richard Löscher[1], Olaf Steinbach[2]

[1] TU Graz

We consider a space-time variational formulation for the wave equation, applying integration by parts also in time and inserting a transformation operator acting on the test functions. This leads to the same ansatz and test spaces and further - using a conforming discretisation - to a Galerkin-Bubnov scheme. This scheme has been analysed by Steinbach and Zank [1] and was found to underly a CFL-condition. Although, a stabilization for a tensor product structure, leading to an unconditionally stable scheme, is available (see [2]), for simplicial space-time meshes this condition has not yet been overcome. In this talk, we give an overview on different approaches to stabilise the scheme on triangular meshes in the space-time domain and their numerical analysis.

References

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This presentation is scheduled for Thursday, 5 May 2022, 15:40.

Finite Element Approximation of Holomorphic Eigenvalue Problems

Martin Halla[1]

[1] Georg-August Universität Göttingen

We consider eigenvalue problems for holomorphic operator functions. We present a framework [1] to conduct the convergence analysis of Galerkin approximatins for such problems. The analysis applies [5] and is based on the notion of weak T-coercivity. We show several examples of application of this framework including perfectly matched layer formulations of scalar resonance problems [2], modified Maxwell Steklov eigenvalue problems [3] and Maxwell transmission eigenvalue problems in dispersive materials [4].

References

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[2] Halla: Analysis of Radial Complex Scaling methods: Scalar Resonance Problems. SIAM J. Numer. Anal., 59, No. 4 (2021), 2054–2074.

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This presentation is scheduled for Thursday, 5 May 2022, 16:30.

Adaptive Magnus-type integrators for the simulation of solar cells

Othmar Koch[1], W. Auzinger[2], K. Held[2], A. Kauch[2], C. Watzenböck[2]

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[2] TU Wien, Wiedner Hauptstraße 8–10, A-1040 Wien

We present adaptive time integrators for large systems of linear homogeneous Schrödinger-type ODEs

$$\mathrm{i}\dot{\psi}(t) = H(t)\psi(t),$$

with an Hermitian matrix $H(t)$, which results from spatial discretization for example based on Wannier functions. One motivation for studying such systems is the simulation of novel oxide solar cells which promise gains in the efficiency of energy conversion. A favorable approach for the numerical solution of such problems is given by commutator-free Magnus-type methods. The oscillatory and rapidly attenuating electric field caused by the impact of a photon and almost stationary behavior thereafter call for adaptive choice of the time-steps. As a basis for such a procedure, a defect-based error estimator is constructed and its asymptotical correctness is proven [1]. Moreover, optimal methods are constructed. In each step, an adaptive Lanczos method based on a novel defect-based error estimator is employed for the task of matrix exponentiation [2]. We demonstrate that the adaptive choice of time-steps increases the efficiency while still faithfully reproducing important characterstics of the system such as the energy or mean double occupation in real-world applications [3] and also enables accurate simulations for non-smooth models such as that of a Mott transistor [4].

References

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This presentation is scheduled for Thursday, 5 May 2022, 16:55.

A-posteriori-steered and hp-robust multigrid solvers

Ani Miraçi[1], Jan Papež[2], Dirk Praetorius[1], Julian Streitberger[1], Martin Vohralík[3]

[1] TU Wien, Austria
[2] Institute of Mathematics, Czech Academy of Sciences, Czech Republic
[3] Inria Paris, France

We study a symmetric second-order linear elliptic PDE discretized by piecewise polynomials of arbitrary degree $p \geq 1$. To treat the arising linear system, we propose a geometric multigrid method with zero pre- and one post-smoothing by an overlapping Schwarz (block Jacobi) method [1]. Introducing optimal step sizes which minimize the algebraic error in the level-wise error correction step of multigrid, one obtains an explicit Pythagorean formula for the algebraic error. Importantly, this inherently induces a fully computable a posteriori estimator for the energy norm of the algebraic error. We show the two following results and their equivalence: 1) the solver contracts the algebraic error independently of the polynomial degree p; 2) the estimator represents a two-sided p-robust bound on the algebraic error. The p-robustness results are obtained by carefully applying the results of [1] for one mesh, combined with a multilevel stable decomposition for piecewise affine polynomials of [2]. Moreover, recent developments in [4] allow to prove that a local variant of the solver is robust also with respect to the number of mesh levels used for rate-optimal adaptive-FEM. Finally, we present a variety of numerical tests to confirm the theoretical results and to illustrate the advantages of our approach.

References

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This presentation is scheduled for Thursday, 5 May 2022, 17:20.

Analysis of intrinsic curvature approximations with Regge finite elements

Michael Neunteufel[1], Jay Gopalakrishnan[2], Joachim Schöberl[1], Max Wardetzky[3]

[1] TU Wien
[2] Portland State University
[3] University of Göttingen

The intrinsic curvature of a Riemannian manifold (M, g) is given by the curvature tensor Q. Regge calculus [1] has originally been developed for solving Einstein field equations in general relativity by discretizing the metric tensor g by piece-wise constant metrics and approximating the curvature Q by means of angle deficits. For two-dimensional manifolds, a proof of convergence for curvature using (high-order) Regge finite elements was recently given in [2].

In this talk we present an improved error analysis of [2] obtaining one extra order of convergence and confirm with numerical examples, implemented in the finite element software NGSolve (www.ngsolve.org), that the rates are optimal. Further, an extension of the high-order curvature approximation in three dimensions is presented leading to optimal numerical convergence rates.

References

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[2] Berchenko-Kogan Y. and Gawlik E. S.: Finite element approximation of the Levi-Civita connection and its curvature in two dimensions. arXiv preprint, 2111.02512 (2021).

This presentation is scheduled for Thursday, 5 May 2022, 17:45.

Finite element analysis for topological derivatives of optimization problems subject to a linear PDE constraint

Nepomuk Krenn[1], Peter Gangl[1]

[1] Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences

The topological derivative describes the variation of a shape functional subject to infinitesimal topological perturbation. We start with the analytical derivation of the topological derivative of a certain class of optimization problems subject to a linear PDE constraint by a Lagrangian approach. In this context, a transmission problem has to be solved on an unbounded domain. Numerically, this equation is solved by performing FEM on a truncated domain. We investigate the error of the discrete topological derivative subject to the truncation parameter, the mesh size of the transmission problem and the mesh size used to approximate the original PDE.

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This presentation is scheduled for Thursday, 5 May 2022, 18:10.

Application of topological derivative in discrete material optimiazton

Peter Gangl[1], Nico Nees[2], Michael Stingl[2]

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We consider a discrete material optimization problem where the goal is to find the optimal value of a piecewise constant material coefficient for each triangular element in a finite element mesh so as to maximize a given cost function. Here, the cost function depends on the material distribution via the solution to an elliptic PDE. Following the idea of sequential global programming, one seeks to approximate the solution of the optimization problem by solving a sequence of first order approximations to the original problem. In this talk, we propose and investigate several separable first-order models which approximate the original problem, compare their accuracies and draw a connection between the Sherman-Morrison-Woodbury formula from matrix analysis and the mathematical concept of topological derivatives.

This presentation is scheduled for Friday, 6 May 2022, 9:00.

Analysis for Full Field Photoacoustic Tomography with Variable Sound Speed

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Photoacoustic tomography (PAT) is a non-invasive imaging modality that requires recovering the initial data of the wave equation from certain measurements of the solution outside the object. In the standard PAT measurement setup, the used data consist of time-dependent signals measured on an observation surface. In contrast, the measured data from the recently invented full-field detection technique provide the solution of the wave equation on a spatial domain at a single instant in time. While reconstruction using classical PAT data has been extensively studied, not much is known for the full field PAT problem. In this paper, we build mathematical foundations of the latter problem for variable sound speed and settle its uniqueness and stability. Moreover, we introduce an exact inversion method using time-reversal and study its convergence. Our results demonstrate the suitability of both the full field approach and the proposed time-reversal technique for high resolution photoacoustic imaging.

This presentation is scheduled for Friday, 6 May 2022, 9:25.

A 3D finite element - boundary element coupling method in time domain for the scalar wave equation

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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 $\Omega^c = \mathbb{R}^3 \backslash \Omega$. 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 present an a priori error estimate and conclude the presentation with different numerical examples.

This presentation is scheduled for Friday, 6 May 2022, 9:50.

A Time-Adaptive Fast Multipole Boundary Element Method for the Heat Equation

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We consider a space-time boundary element method for the solution of initial boundary value problems of the heat equation in three spatial dimensions. In particular we deal with tensor product meshes with adaptive decompositions of the considered time interval. We present a related new time-adaptive version of the fast multipole method and apply shared and distributed memory parallelization with respect to space and time. This combination enables fast computations of the space-time method. Finally, we present numerical experiments that demonstrate the benefits of the new method.

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This presentation is scheduled for Friday, 6 May 2022, 10:15.

Rate-optimal goal-oriented adaptive FEM for semilinear elliptic PDEs

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The talk presents our recent work [1]: Let $\mathcal{X} := H_0^1(\Omega)$. For a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$ and given $f, g \in L^2(\Omega)$, we aim to approximate the linear goal quantity

$$G(u) := \int_\Omega gu \, \mathrm{d}x,$$

where $u \in \mathcal{X}$ is the weak solution of the semilinear elliptic PDE

$$-\mathrm{div}(\boldsymbol{A}\nabla u) + b(u) = f \quad \text{in } \Omega \quad \text{subject to} \quad u = 0 \quad \text{on } \partial\Omega. \tag{1}$$

Here, the diffusion matrix $\boldsymbol{A} \in \mathbb{R}^{d\times d}_{\mathrm{sym}}$ is uniformly positive definite, and the smooth nonlinearity $b(\cdot)$ is monotone and satisfies certain growth conditions. The weak formulation of the so-called *primal problem* (1) reads as follows: Find $u \in \mathcal{X}$ such that

$$\langle \boldsymbol{A}\nabla u, \nabla v\rangle + \langle b(u), v\rangle = \langle f, v\rangle \quad \text{for all } v \in \mathcal{X}, \tag{2}$$

where $\langle v, w\rangle := \int_\Omega vw \, \mathrm{d}x$ denotes the $L^2(\Omega)$-scalar product. Existence and uniqueness of the solution $u \in \mathcal{X}$ of (2) follow from the Browder–Minty theorem on monotone operators. For a fixed polynomial degree $m \in \mathbb{N}$, let $\mathcal{X}_H$ be a conforming FEM space. The FEM discretization of (2) reads: Find $u_H \in \mathcal{X}_H$ such that

$$\langle \boldsymbol{A}\nabla u_H, \nabla v_H\rangle + \langle b(u_H), v_H\rangle = \langle f, v_H\rangle \quad \text{for all } v_H \in \mathcal{X}_H.$$

We approximate the goal quantity $G(u)$ by means of the computable quantity $G(u_H)$. The optimal error control of the goal error $G(u) - G(u_H)$ involves the so-called *(practical) dual problem*, which fits into the Lax–Milgram setting: Find $z[u_H] \in \mathcal{X}$ such that

$$\langle \boldsymbol{A}\nabla z[u_H], \nabla v\rangle + \langle b'(u_H) z[u_H], v\rangle = G(v) \quad \text{for all } v \in \mathcal{X}. \tag{3}$$

The FEM discretization (3) reads: Find $z_H[u_H] \in \mathcal{X}_H$ such that

$$\langle \boldsymbol{A}\nabla z_H[u_H], \nabla v_H\rangle + \langle b'(u_H) z_H[u_H], v_H\rangle = G(v_H) \quad \text{for all } v_H \in \mathcal{X}_H.$$

We prove the goal error estimate

$$C^{-1}\,|G(u) - G(u_H)| \le \|u - u_H\|_{\mathcal{X}} \|z[u_H] - z_H[u_H]\|_{\mathcal{X}} + \|u - u_H\|_{\mathcal{X}}^2.$$

Based on residual error estimators, we formulate a goal-oriented adaptive algorithm (GOAFEM), which guarantees convergence and, as the main contribution, optimal algebraic convergence rates.

References

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This presentation is scheduled for Friday, 6 May 2022, 11:10.

An accurate and efficient finite element framework with applications to cardiac electromechanics

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Image-based computational models of cardiac electromechanics are a powerful tool to understand the mechanisms underlying physiological and pathological conditions in cardiac function and to improve diagnosis and therapy planning.

To realize such advanced applications methodological key challenges must be addressed. First, enhanced computational efficiency and robustness is crucial to facilitate model personalization and the simulation of prolonged observation periods. Second, physiological completeness encompassing therapy-relevant mechanisms is needed to endow models with predictive capabilities beyond the mere replication of observations. Third, fiber-reinforced soft biological tissues are typically modeled as hyperelastic, anisotropic, and nearly incompressible materials. However, the finite element analysis of such problems often suffers from severe volumetric locking effects and numerical instabilities.

In this talk, we present different stabilization techniques to overcome volumetric locking phenomena for using stabilized P1–P1 elements. In benchmark problems from the literature, we compare the approach to standard linear elements and show the accuracy and versatility of the methods to simulate nearly and fully incompressible materials. To show the usefulness of the presented methods to clinically relevant problems, we present a 3D electro-mechanical model of the heart that is coupled to a 0D model of the circulatory system. We demonstrate the model's ability to replicate physiological behavior and discuss possible clinical applications.

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This presentation is scheduled for Friday, 6 May 2022, 11:35.

Initial higher-order pressure convergence in unbalanced finite element discretizations of incompressible flow problems

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In incompressible flow systems, pressure and velocity can be approximated for instance via stable or stabilized finite element methods. For equal-order elements, the classical theory predicts a suboptimal pressure convergence, although a higher order is often observed in numerical practice. In the absence of a sound a-priori error analysis, such experimental observations can mislead the selection of finite element spaces for applications. In this context, we present an improved theory having the pressure Schur complement system as an abstract setting, and low-order elements as realization. Our results demonstrate that an initial higher-order pressure convergence may indeed occur under certain conditions, but also that the occurrence and duration of this phenomenon is problem- and discretization-dependent.

References

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This presentation is scheduled for Friday, 6 May 2022, 12:00.

Large Eddy Simulation with Correction (LES-C) – a new class of turbulence models

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A new family of models for fluid flows at high Reynolds numbers, Large Eddy Simulation with Correction (LES-C), has recently been proposed by the authors; it combines the LES approach to turbulence modeling with defect correction methodology. In this talk we will demonstrate that the LES-C models outperform their LES counterparts in a variety of different settings. These include the computation of errors and convergence rates (for problems with known solutions), a benchmark problem of finding maximal drag and lift coefficients, flow past the step, and a 3-D turbulent channel flow problem. We will also discuss the application of LES-C models to coupled Navier-Stokes systems - a fluid-fluid interaction problem and a MagnetoHydroDynamics problem at high Reynolds and magnetic Reynolds numbers.

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This presentation is scheduled for Friday, 6 May 2022, 12:25.