Austrian Numerical Analysis Day 2024, 16 – 17 May 2024

Abstracts

Overview lectures

Herbert Egger (Linz)
Stability, asymptotic analysis, and discretization error estimates for some nonlinear systems of differential equations

Many problems in science and engineering are described by systems of differential equations which typically encode basic physical principles, like conservation of mass, dissipation of energy, production of entropy, etc. A key ingredient for the analysis and numerical approximation of such problems is the stability of solutions with respect to perturbations.

In this talk, we discuss three examples of problems governed by nonlinear partial differential equations which describe the reduction respectively minimization of a governing nonlinear energy functional. The concept of "relative energy" turns out to be a key ingredient for the stability analysis of the problems. We illustrate its systematic use for proving stability and uniqueness of solutions on the continuous and discrete level, for establishing convergence in asymptotic regimes, and for deriving order optimal discretization error estimates.

Michael Feischl (TU Wien)
Adaptive mesh refinement

The ultimate goal of any numerical method is to achieve maximal accuracy with minimal computational cost. This is also the driving motivation behind adaptive mesh refinement algorithms to approximate partial differential equations (PDEs). The goal of adaptivity is to achieve a mathematically guaranteed optimal accuracy vs. work ratio for such problems. We will review the basics of the theory and discuss recent developments.

Olaf Steinbach (TU Graz)
Space-Time Finite Element Methods: Foundations and Applications

In this talk we will review some recent developments in space-time finite element methods for the numerical solution of time-dependent partial differential equations, with the heat and the wave equation as model problems. This includes the formulation in Bochner and anisotropic Sobolev spaces, and using a modified Hilbert transformation for to obtain a (symmetric) and positive definite approximation of the involved time derivatives. Applications are in the direct simulation of electric motors, optimal control and inverse problems, and in the coupling of multiphysics problems.

Contributed talks

Stefan Tyoler (RICAM ÖAW)
Adaptive Multipatch IgA

"In this talk, we propose a new approach for adaptive discretizations in Isogeometric Analysis. In order to avoid the non local refinement of tensor product discretizations in 2D or higher dimensions, we decompose the computational domain into multiple geometrically non-conforming patches. On each of these patches, we set up individual tensor product discretizations. Since we use different grid sizes on each patch we will discuss the treatment of hanging nodes emerging from local refinement to allow coupling of local basis functions across interfaces. Finally, we show some results by employing this method to some adaptive test problems, utilizing a residual a posteriori error estimator and patchwise refinement."

Isogeometric multi-patch C^1-mortar coupling for the biharmonic equation

Thomas Takacs
RICAM, Austrian Academy of Sciences
thomas.takacs@ricam.oeaw.ac.at

In this talk we discuss an isogeometric mortar method for fourth order elliptic problems. In particular we are interested in the discretization of the biharmonic equation on multi-patch domains. Thus the domain is partitioned into patches that are parametrized by tensor-product B-spline mappings. The patch parametrizations are C^0-conforming. We exploit the mortar technique to weakly enforce C^1-continuity across the patch interfaces. In order to obtain discrete inf-sup stability, a particular choice for the Lagrange multiplier space is needed. To be precise, we use as a multiplier space splines of degree reduced by two, w.r.t. the primal spline space, and with merged elements near all patch corners. In this framework, we are able to show optimal a priori error estimates. We also perform numerical tests to validate the theoretical results.

This talk is based on joint work with Andrea Benvenuti, Gabriele Loli (both Università di Pavia, IT) and Giancarlo Sangalli (Università di Pavia & IMATI-CNR, Pavia, IT).

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16-17 May 2024, Innsbruck, Austria

Strang splitting isogeometric analysis for nonlinear systems of convection-diffusion-reaction in developmental biology

Ilham Asmouh*[1], Alexander Ostermann[2]

Institut für Mathematik, Universität Innsbruck, Technikerstraße 13, 6020 Innsbruck, Austria

Keywords: *Modified method of characteristics; Isogeometric analysis; Transport problems; NURBS functions; Activator and inhibitor; Developmental biology.*

The aim of this recent study is to present a new algorithm for the numerical solution of nonlinear convection-diffusion-reaction equations arising from developmental biology. In this algorithm, the modified method of characteristics is combined with Isogeometric analysis (IGA) to construct a stable and highly accurate method. At the interpolation stage, non-uniform rational B-splines (NURBS) are used to update the solution from known values in an L^2 projection framework since the NURBS are known to be not interpolatory. The proposed method maintains the advantages of the modified method of characteristics scheme in reducing the truncation errors and allowing for large CFL numbers in the simulations. On the other hand, the IGA guarantees the exact representation of the geometry of the computational domain even for coarse meshes. The performance of the new isogeometric semi-Lagrangian analysis is demonstrated for a class of advection-diffusion-reaction systems.

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Numerical analysis of polar vortex stability

Yu Zhang[1,2], Tao Cai[1], Othmar Koch[3], Friedrich Kupka[2,4], and Norbert Mauser[2]

[1]Macau Univ. of Science and Technology, Macau, China
[2]Research Platform MMM "Mathematics-Magnetism-Materials" c/o Fak. Mathematik, Univ. Wien, Oskar Morgenstern Platz 1, A-1090 Wien, Austria
[3]Wolfgang Pauli Institute Vienna, c/o Fak. Mathematik, Univ. Wien, Oskar Morgenstern Platz 1, A-1090 Wien, Austria
[4]Univ. of Applied Sciences FH Technikum Wien, Höchstädtplatz 6, A-1200 Wien, Austria

Polar vortices, significant cyclonic circulations near the poles of planetary atmospheres, are instrumental in shaping weather patterns and atmospheric dynamics. While extensively investigated on Earth, similar phenomena have also been observed on other celestial bodies within our solar system. Notably, Venus exhibits a polar dipole pattern with cyclonic circulation at the north pole and anticyclonic circulation at the south pole. On Jupiter, polar cyclones (PC) are surrounded by a ring of circumpolar cyclones (CPC) at each pole, while Saturn, sharing similarities with Jupiter, only harbors a solitary cyclone in its polar regions.

Comprehending the intricacies of polar vortex dynamics is crucial for understanding the underlying atmospheric processes. In this talk, we employ linear stability analysis and solve the associated eigenvalue problems numerically to investigate the influence of planetary rotation frequency and its variability, as well as the characteristics of circumpolar cyclones including their number, location, relative strength, and radius, on the overall stability of the system. Through this analysis, we aim to advance our understanding of polar vortex behavior across planetary atmospheres, contributing to the broader comprehension of planetary meteorology.

This work is partly supported by the Austrian Science Fund (FWF) under the grant P 35485-N.

Hieu Hoang (Innsbruck)
Stabilized finite elements for unique continuation problems

We consider the unique continuation (or data assimilation) problem which recovers a solution to the Laplace equation from possibly noisy data in a subdomain. We introduce a Tikhonov regularized finite element method for this problem. An a priori estimate is obtained for the error in terms of the stabilization parameter, noise level and mesh size. It allows to determine the optimal stabilization parameter for given noise and discretization.

Andrea Scaglioni (TU Wien)
Sparse grid approximation of nonlinear SPDEs: the Landau—Lifshitz—Gilbert equation

We consider the Stochastic Landau-Lifshitz-Gilbert (SLLG) problem as an example of parabolic stochastic PDE (SPDE) driven by Gaussian noise. Beyond being a popular model for magnetic materials immersed in heat baths, the forward uncertainty quantification (UQ) task poses several interesting challenges that did not appear simultaneously in previous works: The equation is strongly nonlinear, time-dependent, and has a non-convex side constraint. We first use the Doss-Sussman transform to transform the SPDE in a random coefficient PDE. We then employ the Lévy-Ciesielski parametrization of the Wiener process to obtain a parametric coefficient PDE. We study the regularity and sparsity properties of the parameter-to-solution map, which features countably many unbounded parameters and low regularity compared to other elliptic and parabolic model problems in UQ. We use a novel technique to establish uniform holomorphic regularity of the parameter-to-solution map based on a Gronwall-type estimate combined with previously known methods that employ the implicit function theorem. This regularity result is used to design a piecewise-polynomial sparse grid approximation through a profit maximization approach. We prove algebraic dimension-independent convergence and validate the result with numerical experiments. If time allows, we discuss the finite element discretization and multi-level approximation.

Felix Engertsberger (Linz)

We consider the numerical analysis and solution of an energy-based magnetic hysteresis model, which is characterized by a convex non-smooth minimization problem involving the magnetic vector potential and the magnetic polarization. Using techniques from convex analysis, we eliminate the magnetic polarization as an internal variable, resulting in a simplified problem with improved regularity properties. We explore the numerical solution of this reduced problem using various iterative methods, including fixed-point iteration and (Quasi-)Newton methods. Simulation results are presented for a typical benchmark problem.

Ruma Maity (Innsbruck)
Bayesian experimental design for head imaging by electrical impedance tomography

Electrical impedance tomography is an imaging modality for deducing information about the conductivity inside a physical body from boundary measurements of current and voltage by a finite number of contact electrodes. This work applies techniques of Bayesian experimental design to the linearized forward model of impedance tomography in order to select optimal positions for the available electrodes. The aim is to place the electrodes so that the conditional probability distribution of the (discretized) conductivity given the electrode measurements is as localized as possible in the sense of the A-optimality criterion of Bayesian experimental design. The algorithm is developed in the computational framework introduced in [1].

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Alexander J. Pfleger (Cern)
Track Reconstruction of High Energy Particles with a Global χ^2 Fitter

The global χ^2 fitter is a method used to fit initial parameters of a particle track. We implement a modern version for the popular tracking framework ACTS. For the fit, we take a series of measurements from a particle detector, weighting them with the resolution of each detector surface. We expect to have 8 degrees of freedom (which we can reduce to 6). However, material effects introduce additional parameters that we need to fit. Since our target systems include inhomogeneous magnetic fields, we minimise the global χ^2 iteratively. We investigate both the computational performance and the physics performance by fitting tracks from different detectors.

Parameter estimation in cardiac biomechanical models based on physics-informed neural networks

Matthias Höfler [1,3], Francesco Regazzoni[4], Stefano Pagani[4], Elias Karabelas[1,2,3], Christoph Augustin[2,3], Alfio Quarteroni[4,5], Gernot Plank[2,3], Gundolf Haase [1,3], Federica Caforio[1,2,3]

[1] Institute of Mathematics and Scientific Computing, NAWI Graz, University of Graz (Austria)
[2] Gottfried Schatz Research Center: Division of Biophysics, Medical University of Graz (Austria)
[3] BioTechMed-Graz, Austria
[4] MOX, Department of Mathematics, Politecnico di Milano (Italy)
[5] Institute of Mathematics, EPFL (Switzerland) (Professor Emeritus)

Biophysical models of the cardiac function are becoming increasingly popular due to their ability to predict patient outcomes and optimise treatment plans. However, the development and personalisation of these models is computationally expensive and requires extensive calibration, making them difficult to apply in clinical settings. In this presentation we study the application of a novel methodology [1] integrating physics-informed neural networks [2] with high-resolution three-dimensional nonlinear cardiac biomechanical models to reconstruct displacement fields and estimate patient-specific biophysical properties (s.a. passive stiffness and active contractility). The physics of the problem is represented by a mathematical model based on time-dependent partial differential equations. Additionally, the learning algorithm incorporates displacement and strain data that can be routinely acquired in clinical settings. Various training methodologies are explored, e.g. different sampling strategies and architectures for the neural networks. The presentation includes a series of benchmark tests that demonstrate the accuracy, robustness, and promising potential of this method for the precise and efficient determination of patient-specific physical properties in nonlinear biomechanical models.

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Philipp Bringmann (TU Wien)
On full linear convergence and optimal complexity of adaptive FEM with inexact solver

(with Michael Feischl, Ani Miraçi, Dirk Praetorius, Julian Streitberger) 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, algorithmically, the 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.

An hp-Adaptive Strategy Based on Locally Predicted Error Reductions

Patrick Bammer[1], *Andreas Schröder*[1] *and Thomas P. Wihler*[2]

[1] Fachbereich Mathematik, Paris Lodron Universität Salzburg, Austria, patrick.bammer@plus.ac.at
[2] Mathematisches Institut, Universität Bern, Sidlerstr. 5, Switzerland

Abstract – In this talk, an hp-adaptive strategy for variational equations associated with self-adjoint elliptic boundary value problems is introduced, which neither relies on classical a posteriori error estimators nor on smoothness indicators to steer the adaptivity. Instead, the approach compares the predicted error reduction that can be expressed in terms of local modifications of the degrees of freedom in the underlying discrete approximation space. The computations related to the proposed prediction strategy involve low-dimensional linear problems that are computationally inexpensive and highly parallelizable. The concept is first presented in an abstract Hilbert space framework, before it is applied to hp-finite element discretizations. Thereby, a constraint coefficient technique allows a highly efficient computation of the predicted error reductions. The applicability and effectiveness of the resulting hp-adaptive strategy is finally illustrated with some numerical examples.

Stability of conforming space-time isogeometric methods for the wave equation

Matteo Ferrari[a], **Sara Fraschini**[a]

[a] University of Vienna, Vienna (Austria)

matteo.ferrari@univie.ac.at

We consider a family of conforming space–time finite element discretizations for the wave equation based on splines of maximal regularity in time. Traditional techniques may require a CFL condition to guarantee stability. Recent works [3], and [2], have introduced unconditionally stable schemes by adding non-consistent penalty terms to the underlying bilinear form. Stability and error analysis have been carried out for lowest order discrete spaces. While higher order methods have shown promising properties through numerical testing, their rigorous analysis was still missing. In [1], we have addressed this stability analysis by studying the properties of the condition number of a family of matrices associated with the time discretization. For each spline order, we have derived explicit estimates of both the CFL condition required in the unstabilized case and the penalty term that minimises the consistency error in the stabilized case. Numerical tests confirm the sharpness of our results.

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Ernst P. Stephan (Hannover)
Time Domain Boundary Elements for Elastodynamics

The solution to the elastodynamic equation in the exterior of a polyhedral domain or a screen exhibits singular behavior from the corners and edges. This behavior implies quasi-optimal estimates for piecewise polynomial approximations of the Dirichlet trace of the solution and the traction. The results are applied to hp and graded versions of the time domain boundary element method for the weakly singular and the hypersingular integral equations. Numerical examples confirm the theoretical results for the Dirichlet and Neumann problems for screens and for polygonal domains in 2d. They exhibit the expected quasi-optimal convergence rates and the singular behavior of the solutions.
The presented results are from the paper: A.Aimi, G.Di Credico, H. Gimperlein, E.P. Stephan, Higher-order time domain boundary elements for elastodynamics – graded meshes and hp-versions, Numer. Math. 154 (2023), 35 - 101.

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Full-field Photoacoustic Tomography with Variable Sound Speed and Attenuation

Richard Kowar[1], Ngoc Do[2], Markus Haltmeier[1], Linh Nguyen[3]
[1]) Department of Mathematics, University of Innsbruck, Technikerstrasse 13, 6020 Innsbruck, Austria
richard.kowar@uibk.ac.at, markus.haltmeier@uibk.ac.at
[2]) Department of Mathematics, Missouri State University, Springfield MO 65897 USA
ngocdo@MissouriState.edu
[3]) Department of Mathematics, University of Idaho, Moscow, ID 83844 USA
lnguyen@uidaho.edu

In the standard photoacoustic tomography (PAT) measurement setup, the data used consist of time-dependent signals measured on an observation surface. In contrast, the measurement data of the recently invented full-field detection technique provides the solution of the wave equation in the spatial domain at a single point in time. While reconstruction using classical PAT data has been extensively studied, not much is known about the full-field PAT problem. In this work, we study full-field photoacoustic tomography with spatially variable sound velocity and spatially variable attenuation. In particular, we reconstruct the initial pressure from 2D projections of the full 3D acoustic pressure distribution at a given time. Numerical simulations are presented for both full angle and limited angle data cases.

Linear multistep methods with Richardson extrapolation

Imre Fekete[a,b]

[a]Department of Network and Data Science, Central European University, Vienna
[b]Institute of Mathematics, ELTE Eötvös Loránd University, Hungary
feketei@ceu.edu

We investigate the application of the well-known Richardson extrapolation (RE) technique to accelerate the convergence of sequences resulting from linear multistep methods (LMMs) for numerically solving initial-value problems of systems of ordinary differential equations. Furthermore, we utilize some advanced versions of RE in the form of repeated global (also known as passive) RE. Assuming that the underlying LMM (the base method) has order p and RE is applied ℓ times, we prove that the accelerated sequence has convergence order $p+\ell$. We also investigate how the linear stability properties (e.g., A- or $A(\alpha)$-stability) of the base method are preserved. At the end of talk we point out some computational aspects of the introduced methods.

This is a joint work with Lajos Lóczi (ELTE Eötvös Loránd University, Hungary and BME Budapest University of Technology and Economics, Hungary).

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Parametric PDEs and low-rank approximation of function-valued matrices

Stanislav Budzinskiy

Faculty of Mathematics, University of Vienna

Parameter tuning for mathematical models relies on massive high-fidelity simulations of the underlying PDEs and becomes more expensive with the growing complexity of the models. The idea of data-driven modeling is to replace the original model with a *surrogate* one that is built based on the results of high-fidelity simulations carried out for a small number of parameter values. In this talk, we present a new framework of data-driven modeling for bi-parametric PDEs. We propose to

(i) treat them, after the discretization of the parameter space, as matrices whose entries are the solutions of the PDE for the corresponding parameter values;

(ii) seek low-rank approximations of such function-valued matrices.

This research is funded by the “Disruptive Innovation – Early Career Seed Money” funding program of the Austrian Academy of Sciences (ÖAW) and the Austrian Science Fund (FWF).

Ignacio Labarca (Innsbruck)
Coupled Boundary and Volume Integral Equations for Electromagnetics

We study frequency domain electromagnetic scattering at a bounded, penetrable, and inhomogeneous obstacle. From the Stratton-Chu integral representation, we derive a new representation formula when constant reference coefficients are given for the interior domain. The resulting integral representation contains the usual layer potentials, but also volume potentials. Then it is possible to follow a single-trace approach to obtain boundary integral equations perturbed by traces of compact volume integral operators with weakly singular kernels. The coupled boundary and volume integral equations are discretized with a Galerkin approach with usual Curl-conforming and Div-conforming finite elements on the boundary and in the volume. Compression techniques and special quadrature rules for singular integrands are required for an efficient and accurate method. Numerical experiments provide evidence that our new formulation enjoys promising properties.

Fabian Zehetgruber (TU Wien)
An implicit function theorem for neural networks

The classical method to understand how well the solutions of parametric PDEs can be approximated using artificial neural networks employs regularity theory. Since regularity results are sparse for nonlinear PDEs, we aim to bypass this bottleneck by studying neural networks in connection with the implicit function theorem. We investigate if an implicitly given set of points that can be described by the realization of a neural network can locally be well approximated as the graph of the realization of another neural network. In addition to the mere existence of such an approximation we obtain bounds on the number of nodes and the depth of the approximating neural network. Mathematically, this requires a precise understanding of sums and compositions of neural networks.

Stefan Takacs (Linz)
High-order isogeometric and finite element discretizations for elasticity problems

(with Jarle Sogn) We consider the discretization of the linearized elasticity equation. A standard discretization error analysis is based on Korn's inequality. The constant introduced by Korn's inequality analysis degrades for certain geometries, like long and thin cantilevers. Additionally, the overall error bound for the discretization error degrades for incompressible and almost incompressible materials. In numerical experiments, one can observe that high-order methods are beneficial in such a setting. While this fact is well-known in literature, the theoretical understanding is much more limited. A recent paper gave a theoretical explanation why high order methods are beneficial for the discretization the primal formulation of elasticity problems for almost incompressible materials. We will discuss why high order methods are beneficial for the discretization of elasticity problems on long and thin geometries, like cantilevers.

Michael Winkler (Linz)
Continuation methods for higher-order density-based topology optimization

We aim to solve a topology optimization problem where the distribution of material in the design domain is represented by a density function. To obtain candidates for local minima, we want to solve the first order optimality system via Newton's method. This requires the initial guess to be sufficiently close to the a priori unknown solution. Introducing a stepsize rule often allows for less restrictions on the initial guess while still preserving convergence. In topology optimization one typically encounters nonconvex problems where this approach might fail. We therefore opt for a homotopy (continuation) approach which was first introduced in the 1980s and is based on solving a sequence of parameterized problems to approach the solution of the original problem. The arising Newton-type method also allows for employing deflation techniques for finding multiple distinct solutions. We finally show first numerical results.