42^{ND} NORTHERN GERMAN COLLOQUIUM ON APPLIED ANALYSIS AND NUMERICAL MATHEMATICS

Institut für Mathematik

Carl von Ossietzky Universität Oldenburg

June 28–29, 2024

Organizers: Alexey Chernov, Hannes Uecker, Frank Schöpfer, Tung Le, Alexander Meiners

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Poster	Boris Gulyak	Willmore energy for graphs on bounded domains
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09:30	Carolin Mehlmann	Analysis of a nonconforming finite element method for vector-valued geophysical flow problems
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11:00	Bernhard Endtmayer	Homotopy: Following the path to the solution
11:30	Abhishek Kumar	Fractional Orthogonal Polynomials: Diverse Applications and Insights
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Friday 28.06.2024, 13:00

A consistent multi-species BGK model with velocity dependent collision frequencies.

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Rarefied gas dynamics is usually described by the Boltzmann equation. Unfortunately, the expense of evaluating this operator can be very prohibitive. This made it worthwhile to look for approximations that convey essentially an equivalent amount of physical information. One widely known approximative collision operator is the Bathnagar-Gross-Krook (BGK) operator. However, there are some drawbacks. One is that the model assumes that collision frequencies are independent of the microscopic velocity of the particles. In this talk, we present a multi-species BGK model with velocity-dependent collision frequency for a non-reactive, multi-component gas mixture. The model is derived by minimizing a weighted entropy under the constraint that the number of particles of each species, total momentum, and total energy are conserved. We show that this minimization problem admits a unique solution for very general collision frequencies. Moreover, we prove that the model satisfies an H-Theorem and characterize the form of equilibrium and present a numerical method for simulating this model, which uses an Implicit-Explicit (IMEX) scheme to minimize a certain potential function, mimicking the Lagrange functional that appears in the theoretical derivation. We show that theoretical properties such as conservation of mass, total momentum and total energy as well as positivity of the distribution functions are preserved by the numerical method, and illustrate its usefulness and effectiveness with numerical examples.

Friday 28.06.2024, 13:30

Simulating water flows: challenges and solutions

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Simulating water flows accurately presents numerous challenges, particularly in maintaining the positivity of certain quantities and ensuring conservation. Modified Patankar schemes have emerged as a powerful tool to address these issues, capable of preserving positivity in production-destruction systems (PDS) regardless of time step size. These schemes have proven effective in various applications, from solving biological and chemical systems to serving as robust time integrators in the semi-discretization of hyperbolic balance laws. This presentation introduces the fundamentals of modified Patankar methods and highlights their application in creating high-order, well-balanced, and unconditionally positivity-preserving methods for flood simulations.

Friday 28.06.2024, 14:00

Modelling, simulation and optimisation of a SWRO-PRO hybrid system

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Reverse osmosis (RO) is the most widely used membrane based desalination technology. However, it still requires a lot of energy to produce freshwater. The highly concentrated rejected solution of the RO process can be used for Pressure retarded osmosis (PRO). Therefore, a RO-PRO hybrid system could potentially reduce the specific energy consumption (SEC) of the system. In this work we are modelling a membrane unit for both RO and PRO. The mathematical model describes the important flow quantities along the length of the membrane. For a realistic approximation, we include internal concentration polarization (ICP) and external concentration polarization (ECP) effects. Together with a model for a modern Energy recovery device (ERD), we are able to implement and simulate the RO-PRO hybrid system. Finally, we optimize the operating pressures of a conventional RO system and the operating conditions of a hybrid system.

Poster

Modelling a Reverse Electrodialysis Power Plant

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Reverse electrodialysis (RED) is a way of harvesting energy from the salinity difference of a high concentrated solution and low concentrated solution, for example salt and fresh water or brine and brackish water. In this poster, we present a mathematical model for a system of first order nonlinear ODEs describing this phenomenon.

Poster

Willmore energy for graphs on bounded domains

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We present the study of Willmore energy for surfaces with clamped boundaries embedded in $\mathbb{R}^3$, which can be expressed as graphs of real functions defined on a bounded domain in $\mathbb{R}^2$. These surfaces are embedded in $\mathbb{R}^3$ and projected onto $\mathbb{R}^2$ at the same time. In physics, the Willmore energy of a surface quantifies contributions from its stiffness, while geometrically, it sums the square of the curvature resulting from the surface's embedding into $\mathbb{R}^3$. Our primary goal is to identify and characterize the critical points of the Willmore functional, known as Willmore surfaces, which solve the Euler-Lagrange equation, referred to as the Willmore equation. Reformulated for graph functions, this fourth-order elliptic boundary value problem features a Δ^2 operator with a nonlinear divergence right-hand side. This approach leverages explicit coordinates to analytically demonstrate the existence of smooth interior solutions, provided the $C^{1+\alpha}$ norm of the Dirichlet boundary data is sufficiently small, using linearization techniques. Additionally, we explore the gradient flow of the Willmore functional, known as the Willmore flow, which corresponds to a fourth-order parabolic problem with smoothing properties. We establish analytical short-time existence for initial data with C^1 smoothness and Dirichlet boundary data with $C^{4+\alpha}$ regularity. For sufficiently small data, we also demonstrate long-time existence with convergence toward a critical point. Finally, we mention the compactness properties of Willmore minimal sequences within the framework of varifolds or BV spaces, where the appearance of a Cantor part with finite Willmore energy was observed. Notably, for steeper boundary values, numerical experiments indicate a potential loss of projectability during minimization processes. Additionally, some bifurcation phenomena appear for Willmore surfaces of revolution.

Friday 28.06.2024, 15:00

Multi-fidelity learning for light harvesting complexes

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The molecular simulation of light harvesting complexes, i.e. systems of molecules that react on light, such as in photosynthesis or solar cells, is very computationally challenging. Multi-scale methods reduce the computational burden, however highly accurate quantum chemistry calculations in larger complexes are computationally infeasible. In the talk, we present approaches to replace some of the computationally challenging calculations by kernel-based or Gaussian process regression models. Since even the construction of appropriate training sets may become computationally intractable, we develop multi-fidelity techniques to optimally combine training data that has been generated with different accuracies. Practical examples show that this can lead to substantial cost reductions.

Friday 28.06.2024, 15:30

Quasi-Monte Carlo methods for Bayesian design of experiment problems governed by parametric PDEs

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Joint work with:
Claudia Schillings (FU Berlin)

The goal in Bayesian optimal experimental design (OED) is to maximize the expected information gain for the reconstruction of unknown quantities in an experiment by optimizing the placement of measurements. The objective function in the resulting optimization problem involves a multivariate double integral over the high-dimensional parameter and data domains. For the efficient approximation of these integrals, we consider two approaches: a full tensor product and a sparse tensor product combination of quasi-Monte Carlo (QMC) cubature rules over the parameter and data domains. Specifically, we show that the latter approach significantly improves the convergence rate, exhibiting performance comparable to that of QMC integration of a single high-dimensional integral. Furthermore, we numerically verify the predicted convergence rates for an elliptic PDE problem with an unknown diffusion coefficient, offering empirical evidence supporting the theoretical results.

References

V. Kaarnioja and C. Schillings. *Quasi-Monte Carlo for Bayesian design of experiment problems governed by parametric PDEs.* Preprint 2024, arXiv:2405.03529 [math.NA]

Friday 28.06.2024, 16:00

Parametric regularity for the Navier-Stokes problem

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Joint work with:
Alexey Chernov (Universität Oldenburg)

We investigate a class of parametric unsteady incompressible Navier-Stokes equations, where the coefficients (hence the velocity field and the pressure) may depend on high-dimension parameter. For the efficient approximate evaluation of parameter sensitivities of the solution on the entire parameter space we propose and analyse Gevrey class and analytic regularity of the solution with respect to the parameters. In this talk, we introduce a novel proof technique, namely alternative-to-factorial, and demonstrate that the parametric regularity of the solution inherits from the regularity of input data. Our regularity result has immediate implications for convergence of various numerical schemes e.g. integration by generalized polynomial chaos, Quasi-Monte Carlo methods.

References

Alexey Chernov, Tung Le, *Analytic and Gevrey class regularity for parametric semilinear reaction-diffusion problems and applications in uncertainty quantification*, Comput. Math. Appl., 15 June 2024, Vol. 164, pg. 116-130.

Alexey Chernov, Tung Le, *Analytic and Gevrey class regularity for parametric elliptic eigenvalue problems*, SIAM J. Numer. Anal., accepted 2024, Arxiv preprint, https://arxiv.org/pdf/2306.07010.

Friday 28.06.2024, 17:00

Guaranteed lower eigenvalue bounds for the Schrödinger eigenvalue problem

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Joint work with:
Carsten Carstensen (HU Berlin)

This presentation derives several novel guaranteed lower eigenvalue bounds (GLB) for the linear Schrödinger eigenvalue problem $-\Delta u + \gamma u = \lambda u$, $\gamma \in L^\infty(\Omega; [0, \infty))$.

The first part of the presentation discusses GLB by the lowest-order nonconforming CrouzeixRaviart and enriched Crouzeix-Raviart FEM as a generalization of the post-processing techniques in [1]. The second part discusses a modified enriched Crouzeix-Raviart scheme that leads to $\|\gamma\|_\infty$-robust GLB and an extra-stabilized scheme that even allows for direct GLB, both for piecewise constant potential γ.

Numerical experiments in 2D confirm the GLB and their convergence to the exact eigenvalues for various domains and potential regimes. The numerical examples highlight that the modified enriched Crouzeix-Raviart scheme leads to sharper GLB than a recent approach with mixed FEM in [3].

References

[1] C. Carstensen and J. Gedicke, *Guaranteed lower bounds for eigenvalues,* Math. Comp., 83(290):2605–2629, 2014.

[2] C. Carstensen and S. Puttkammer, *Adaptive guaranteed lower eigenvalue bounds with optimal convergence rates,* Numer. Math., 156:1–38, 2024.

[3] D. Gallistl, *Mixed methods and lower eigenvalue bounds,* Math. Comp., 92(342):1491–1509, 2023.

Friday 28.06.2024, 17:30

Quantum Linear Systems Algorithms applied to Partial Differential Equations with Poisson's problem as an example

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Quantum Linear Systems Algorithms (QLSAs) promise an exponential speedup over any classical algorithm for solving sparse linear systems of equations. To obtain this speedup, the problem formulation is restricted to only ask for a scalar function of the solution vector. We study the QLSA by Childs, Kothari and Somma which has a dependence of $O(poly(log(\varepsilon))$ on the precision ε, an exponential improvement over the HHL (Harrow, Hassidim & Lloyd) algorithm. As an example application, we consider the Poisson problem on a 2D grid. Using a matrix-free numerical simulation of the full quantum state vector, we successfully obtain approximations of various objective functionals such as line integrals. Our results show that the algorithm gives promising results even with a few hundred qubits, while scaling well to larger numbers of qubits.

Saturday 29.06.2024, 9:00

GPU Acceleration of a General Purpose Finite Element Framework

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Joint work with:
Utku Kaya, Christian Lessig, Manuel Liebchen

Even though GPUs have been included as accelerator hardware in almost all computers, from laptops and workstations to powerful supercomputers, they have so far been used very little in the context of finite element simulations. This is due to the fact that their programming partly follows paradigms that stand in the way of efficient adaptive finite element methods. As a result, a large part of the available computer power remains unused. In this talk we describe the embedding of GPU's as accelerators in the geometric multigrid solver used by the finite element library Gascoigne. In this talk we describe the embedding of GPU's as accelerators in the geometric multigrid solver used by the finite element library Gascoigne. Special attention is paid to an implementation that is equally efficient and requires only minimal changes to the library.

For this purpose, all operations of the multigrid method, but also the treatment of locally refined grids with hanging nodes is based on matrix-vector multiplications. This approach is standard in the literature. Porting to the GPU is then carried out using the cuSparse library. Particular attention is paid to avoiding memory transfers between the CPU and GPU.

We present various numerical examples and discuss the performance and also the limitations of the methodology. The efficiency of the methods implemented so far strongly depends on the formulation of the whole process based on matrix-vector products. This is a major limitation in the treatment of general nonlinear problems. Nevertheless, we will demonstrate for the Navier-Stokes equations that an acceleration by a factor of 30 can be achieved compared to multicore systems.

Saturday 29.06.2024, 9:30

Analysis of a nonconforming finite element method for vector-valued geophysical flow problems

Carolin Mehlmann

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We analyze a recently developed nonconforming surface finite element which is used to discretize 2D vector-valued compressible geophysical flow problems in a 3D domain. The study is performed on a vector-valued Laplace problem, which results from modeling surface flows. In our approach, the flow is approximated via edge integration on local flat triangles using the nonconforming linear Crouzeix-Raviart element. The approach is numerically efficient and straightforward to implement. For this discretization we derive optimal error bounds and present an estimate for the geometrical error. Numerical experiments validate the theoretical results. Furthermore, we demonstrate that the non-conforming finite element discretization provides a stable realization of large-scale geophysical flow problem.

Saturday 29.06.2024, 10:00

Modeling measurement procedures

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The aim of a measurement is to quantify a previously defined concept. In general, repeated measurements lead to different results and we refer to this random component as aleatory uncertainties. In comparison with other measurement procedures, systematic differences are noticeable. We refer to the systematic effects as epistemic measurement errors.

For study purpose, we introduce a conceptual framework that allows the analysis of measurements from a fully informed perspective. The framework starts with a quantity χ in the reality, which is assumed to be at least theoretically accessible, describable and quantifiable. Then, the concept u and the idealized measurement result w_M for vanishing uncertainties are determined by χ. Within the framework, it is now possible to define the epistemic error as the difference between u and w_M.

Real measurements take the data-centered perspective in which the concept is not accessible. Instead, there might be an established but expensive high-fidelity (HiFi) measurement procedure as a reference for the low-fildelity (LoFi) measurement under consideration. The task of calibrating the LoFi measurement is to find a mapping of the idealized measurement result to the idealized HiFi result.

We illustrate the modeling framework by means of measurements of high-frequent voltages with sampling oscilloscopes

Saturday 29.06.2024, 11:00

Homotopy: Following the path to the solution

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In this work, we present the basic idea of homotopy methods or continuation method. In many applications, second order methods like Newton do not converge, if no 'good initial guess is known. Here, we use a path following technqiue driven by a predictor corrector method. Finally, we apply the technique to shape optimization problems.

Saturday 29.06.2024, 11:30

Fractional Orthogonal Polynomials: Diverse Applications and Insights

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We encounter fractional orthogonal polynomials in the literature, which have one additional degree of freedom compared to the classical orthogonal polynomials. A class of fractional orthogonal polynomials consists of Müntz-Legendre polynomials. Müntz-Legendre polynomials are orthogonal with respect to weight function $W(x) = 1$. However, in practical scenarios where data exhibit varying levels of accuracy or significance across different regions, a constant weight function may not be the best choice. Thus, we discuss how to generate the fractional orthogonal polynomials with respect to general weight functions in discrete as well as continuous cases. Fractional orthogonal polynomials have demonstrated their utility in practical applications across various fields. For instance, they are particularly effective in solving fractional differential equations, which are common in modeling memory and hereditary properties of different materials and processes. Additionally, fractional orthogonal polynomials are vital in curve fitting, especially using the linear least squares method, where they help achieve more accurate fitting results. Another important application is in numerical integration, where these polynomials can improve the accuracy and efficiency of integral approximations.

An embedded trace theorem for infinite metric trees with applications to transmission problems with mixed dimensions

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Joint work with:
Valentina Franceschi (Padova), Maryna Kachanovska (Paris) and Konstantin Pankrashkin (Oldenburg).

For a class of weighted infinite metric trees we propose a definition of the boundary trace which maps H^1-functions on the tree to L^2-functions on a compact Riemannian manifold. For a range of parameters, the precise Sobolev regularity of the traces is determined. This allows one to show the well-posedness for a Laplace-type equation on infinite trees interacting with Euclidean domains through the boundary. Based on joint works with Valentina Franceschi (Padova), Maryna Kachanovska (Paris) and Konstantin Pankrashkin (Oldenburg).