30th Biennial Conference on Numerical Analysis

24 – 27 June, 2025

Contents

Invited Speakers

Erik Burman	University College London	e.burman@ucl.ac.uk
Nicolas Gillis	University of Mons	nicolas.gillis@umons.ac.be
Jacek Gondzio	University of Edinburgh	j.gondzio@ed.ac.uk
Roland Herzog	Heidelberg University	roland.herzog@iwr.uni-heidelberg.de
Buyang Li	Hong Kong Polytechnic University	buyang.li@polyu.edu.hk
Xiaoye Sherry Li	Lawrence Berkeley National Laboratory	xsli@lbl.gov
Mária Lukácová	Johannes Gutenberg-University Mainz	lukacova@uni-mainz.de
Fabio Nobile	École Polytechnique Fédérale de Lausanne	fabio.nobile@epfl.ch
Marie E Rognes	Simula Research Laboratory	meg@simula.no
Katharina Schratz	Sorbonne University	katharina.schratz@sorbonne-universite.fr
Alex Townsend	Cornell University	townsend@cornell.edu
Andy Wathen	University of Oxford	andrew.wathen@stfc.ac.uk

Abstracts of Invited Talks

Computational Unique Continuation

Erik Burman *(University College London)*

The problem of extending measured data from a limited observation region to a larger domain, subject to a governing partial differential equation (PDE), is known as a unique continuation problem. Such problems arise frequently in data assimilation, inverse problems and control theory. They are typically **severely ill-posed**, making their accurate numerical approximation particularly challenging.

In this talk, we present recent advances in the finite element approximation of unique continuation problems. We place special emphasis on the interplay between **physical stability** (inherent to the PDE) and **numerical stability** (introduced by discretisation). This tension motivates a critical reassessment of classical approaches, such as Tikhonov regularisation applied at the continuous level prior to discretisation.

We introduce a novel computational framework that integrates numerical stability with the conditional stability of the underlying physical problem. This approach yields approximations that are provably optimal under certain conditions. We conclude by exploring several variants and applications of the method, supported by computational illustrations.

Nonnegative Tucker Decomposition: Introduction, Identifiability and Algorithms

Nicolas Gillis & Subhayan Saha, Giovanni Barbarino *(University of Mons)*

Tensor decompositions have become a central tool in data science, with applications in areas such as data analysis, signal processing, and machine learning. A key property of many tensor decompositions, such as the canonical polyadic decomposition, is identifiability, that is, the factors are unique, up to trivial scaling and permutation ambiguities. This allows one to recover the groundtruth sources that generated the data. The Tucker decomposition (TD) is a central and widely used tensor decomposition model. However, it is in general not identifiable. In this talk, we first introduce and motivate matrix and tensor decomposition models, with a focus on nonnegative matrix factorization (NMF) and nonnegative Tucker decomposition (NTD). Then, we study the identifiability of NTD. For order-2 tensors, that is, matrices, NTD is equivalent to a nonnegative tri-factorization model. By adapting and extending identifiability results of NMF, we provide uniqueness results for order-2 NTD. The conditions require the nonnegative matrix factors to have some degree of sparsity (namely, satisfy the sufficiently scattered condition), while the core matrix only needs to be full rank. We extend the result to order-3 tensors, which requires the nonnegative matrix factors to satisfy the same sufficiently scattered condition, while the core tensor only needs to have some slices (or linear combinations of them) or unfoldings with full column rank. We also discuss how this result can be extended to higher-order tensors. Finally, we propose an efficient algorithm to compute these unique NTDs, which we illustrate on synthetic and real data.

Nonlinear Techniques to Solve Linear Optimization Problems: Think of Interior Point Methods

Jacek Gondzio *(University of Edinburgh)*

Roger Fletcher and Michael Powell made groundbreaking contributions to the theory and practice of numerical linear algebra and optimization. In this lecture, I will recall some of their seminal works which launched the field of nonlinear optimization. I will also talk about interior point methods. Their development started from a somewhat surprising use of a *nonlinear* technique (logarithmic barrier) in the context of *linear* optimization. Later this led to establishing a class of very successful methods which deal with linear, quadratic, nonlinear and semidefinite optimization and excel at solving large problems. The legacy of Fletcher and Powell continues to have an impact on a broad area of optimization. I will illustrate it with a very recent application of a quasi-Newton technique in the context of interior point methods.

Krylov Subspace Methods with a Twist

Roland Herzog *(Heidelberg University)*

Krylov subspace methods are widely used iterative solvers for real or complex linear systems. In this talk, I will advocate that these methods should be viewed as more than just algorithms juggling matrices and vectors. Instead, with a view towards the setting behind the linear systems, we will systematically re-derive a general residual minimizing Krylov subspace method. This leads to a more general view on and implementation of GMRES and further surprises.

Challenges, numerical analysis, and new computational methods for geometric flows and moving interface problems

Buyang Li *(The Hong Kong Polytechnic University)*

We discuss some key challenges in the numerical analysis of geometric flows and free boundary problems in fluid dynamics. Then we present recent advances in the numerical analysis and algorithmic design for solving these complex and evolving systems. Topics include the convergence of finite element methods for mean curvature flow, the convergence of interface tracking methods for two-phase flows, and the design of artificial tangential motions to improve mesh quality in the computation of evolving surfaces.

Fast Construction of Hierarchically Low-Rank Matrices Using Randomized Sketching

Xiaoye Sherry Li *(Lawrence Berkeley National Laboratory)*

Hierarchically low-rank (H-LR) matrices have been widely used to design fast solvers for integral equations, boundary element methods, discretized PDEs, and kernel matrices in statistical and machine learning. These matrices include H/H2-matrices, HODLR matrices, HSS matrices and butterfly matrices. They differ in the treatment of the off-diagonal low-rank structures. These matrices can be used in iterative solvers where stuctured-matrix-vector-product is needed, or in direct solvers where structured-factorization and stuctured-solve are needed. The computational bottleneck in these types of solvers is often the construction algorithm which converts a standard dense matrix into an H-LR format. The dense matrix may not be explicitly stored. In recent advances of this field, we have seen extensive use of randomized sketching to speed up the construction process. Regardless of which H-LR formats, the common questions include: 1) which random matrix to use? 2) what size of the random matrix to use? 3) what are the error bounds of the H-LR approximation? 4) what are the key ingredients needed for high performance implementations? We will present a unified view to answer these questions, illustrate the algorithms on various applications, and discuss some open problems.

Numerical analysis of oscillatory solutions of compressible flows

Mária Lukáčová-Medvid'ová *(University of Mainz)*

Oscillatory solutions of compressible flows arise in many practical situations, e.g. in shear flows. An iconic example is the Kelvin-Helmholtz problem, where standard numerical methods yield oscillatory solutions. In such a situation, standard tools of numerical analysis for partial differential equations are not applicable. We will show that structure-preserving numerical methods converge in general to generalized solutions, the so-called dissipative solutions. The latter describe the limits of oscillatory sequences. We will concentrate on the inviscid flows, the Euler equations, and mention also the relevant results obtained for the viscous compressible flows, governed by the Navier-Stokes equations.

In the case that the strong solution to the above equations exists, the dissipative solutions coincide with the strong solution on its life span. Otherwise, we apply a newly developed concept of $\mathcal{K}$-convergence and prove the strong convergence of the empirical means of numerical solutions to a dissipative solution. The latter is the expected value of the dissipative measure-valued solutions and satisfies a weak formulation of the Euler equations modulo the Reynolds turbulent stress. If time permits, we will also derive error estimates for the corresponding finite volume method. The error analysis is realized by means of the relative energy which is a problem-suited "metric". We will also discuss a relation between numerical approximations of oscillatory solutions and the Dafermos criterion on maximization of the entropy production. Theoretical results will be illustrated by a series of numerical simulations.

Iterative and multilevel methods for PDE-constrained optimization under uncertainty

Fabio Nobile & Tommaso Vanzan *(Ecole Polytechnique Fédérale de Lausanne)*

In this talk we consider Optimal Control Problems (OCPs) constrained by random Partial Differential Equations (PDEs), where an optimal (deterministic) forcing term is sought so as to minimize the expected value or other risk measures of a cost functional. We will first focus on iterative methods to solve the optimality system associated to the OCP once the underlying PDE and the probability space have been suitably discretized. Such optimality system is typically of very high dimension, characterized by a coupled system of N state PDEs, N adjoint PDEs, and a single optimality condition, where N is the number of collocation points used to discretize the probability space. We present few preconditioning and multigrid strategies to solve efficiently the coupled optimality system and test them on several cases, including an OCP with box constraints and L^1 penalization on the control, and a risk-adverse OCP involving the smoothed CVaR risk measure. We then discuss how multilevel ideas and hierarchical approximations can be used in the the context of PDE-constrained OCPs under un-

certainty adopting a combination technique approach, which requires solving the OCP for several low-fidelity discretizations of the PDE and quadrature formulae to compute the expected cost functional. All the computed solutions are then linearly combined to get a final approximation. We show some theoretical error estimates and present numerical results showing the efficacy of the approach.

References

[1] F. Nobile and T. Vanzan, Multilevel quadrature formulae for the optimal control of random PDEs, July 2024, Available as arXiv:2407.06678.

[2] F. Nobile and T. Vanzan, A combination technique for optimal control problems constrained by random PDEs, SIAM J. Uncert. Quant. 12(2), p. 693–721, 2024. Doi: 10.1137/22M1532263.

[3] G. Ciaramella, F. Nobile and T. Vanzan, A multigrid solver for PDE-constrained optimization with uncertain inputs, J. Sci Comput, 101, article 13, 2024. Doi: 10.1007/s10915-024-02646-7.

[4] F. Nobile and T. Vanzan, Preconditioners for robust optimal control problems under uncertainty, Num. Lin. Algebra with Appls. 30(2), p. e2472, 2023. Doi: 10.1002/nla.2472S.

Brain membranes and vasculature: a computational mathematics tale of dimensional gaps

Marie E. Rognes *(Simula Research Laboratory)*

Structurally, brain tissue is characterized by thin cell membranes and slender vessels, defining submanifolds of codimension one and two respectively. Functionally, your brain fundamentally relies on the transport of ions and nutrients and movement of water in and between these spaces. These physiological processes are clearly crucial for brain function and health, but the precise mechanisms and their association with neurodegenerative diseases such as Alzheimer's and Parkinson's disease and neurological events such as seizures remain only partially understood. Notably, mathematical and computational modelling are beginning to play an important role in gaining new insight. In this talk, I will discuss key mathematical, numerical and computational challenges associated with modelling brain mechanics and transport across scales with an emphasis on coupled systems of partial differential equations with dimensional gaps.

Resonances as a computational tool

Katharina Schratz *(Sorbonne Université)*

A large toolbox of numerical schemes for dispersive equations has been established, based on different discretization techniques such as discretizing the variation-of-constants formula (e.g., exponential integrators) or splitting the full equation into a series of simpler subproblems (e.g., splitting methods). In many situations these classical schemes allow a precise and efficient approximation. This, however, drastically changes whenever non-smooth phenomena enter the scene such as for problems at low regularity and high oscillations. Classical schemes fail to capture the oscillatory nature of the solution, and this may lead to severe instabilities and loss of convergence. In this talk I present a new class of resonance based schemes. The key idea in the construction of the new schemes is to tackle and deeply embed the underlying nonlinear structure of resonances into the numerical discretization. As in the continuous case, these terms are central to structure preservation and offer the new schemes strong geometric properties at low regularity.

I will present the key idea behind resonances as a computational tool, their high order counterpart (via tree series inspired by singular SPDEs), their error estimates in low regularity spaces (via discrete Bourgain spaces) and numerical experiments on nonlinear dispersive quantization effects. I also want to address the fundamental question of resonance based schemes and structure preservation, i.e., central symmetries and even more so symplecticity.

A Mathematical Guide to Operator Learning

Alex Townsend *(Cornell University)*

A fundamental challenge in modern scientific computing is learning an operator from finite data. In this talk, we offer a mathematical guide to operator learning, drawing a distinction between passive and active observation models and revealing the crucial role this choice plays in sample efficiency. We explore how the nature of the underlying partial differential equation, i.e., elliptic, parabolic, or hyperbolic, governs the difficulty of learning the associated solution operator, and we present recent learning theory that quantifies the number of queries needed for accurate recovery. Diffusive systems, as we shall see, are forgiving; wave-like systems are not. Along the way, we reflect on what it means to learn in infinite dimensions and how mathematical structure can be exploited to tame the curse of dimensionality.

Preconditioning and iteration for linear systems

Andy Wathen *(Rutherford Appleton Laboratory)*

Preconditioned iteration has enabled the solution of many problems of huge dimension. In this talk, I will reflect on the art of preconditioning and discuss the requirements and convergence of the most common Krylov subspace iterative solution methods: Conjugate Gradients, MINRES and GMRES.

Minisymposia abstracts

Minisymposium M1

Numerical Methods for Surface and Interface Dynamics
Organisers
Buyang Li and Rong Tang

Higher Order Unfitted Space-Time Methods for moving domain problems

Fabian Heimann *(University College London)* & Christoph Lehrenfeld *(University of Göttingen)* & Janosch Preuss *(Inria Bordeaux - Sud-Ouest)*

Finite Element (FE) methods are a well-established tool for solving partial differential equations. In recent years, Unfitted Finite Elements have been developed around the idea that complex computational domains could be represented implicitly against a fixed background mesh. In this talk, we focus on moving domain problems of advection-diffusion type and present recent results on the convergence of higher order space time methods. The physical summands in the involved bilinear forms follow the standard space time FE paradigm, and a direct volumetric space-time Ghost penalty is applied to maintain numerical stability in the presence of small cuts. Moreover, upwind type jump penalty terms allow for a convenient Discontinuous Galerkin in time discretisation.

In the context of a moving domain bulk problem, we start to investigate the convergence of the salient methods numerically. For a manufactured solution setup in up to 3 spatial dimensions, optimal order convergence is shown for polynomial space orders such as $k = 1, \dots, 6$. We sketch some insights into how this convergence behaviour can also be proven in a strict mathematical sense. To this end, the error incurred by the discrete geometries is first bounded. This can be seen as a generalisation of results on higher order isoparametric Unfitted Finite Elements to the space-time case. Next, these results are used in a discretisation error analysis, which yields bounds on the overall error by establishing inf-sup stability and bounding the resulting error summands from a corresponding proof of the structure of Strang's second lemma.

To broaden the range of application of these methods, we present numerical results on a coupled problem as well, where advection-diffusion processes are included both in surface and bulk of an unfitted moving geometry, and linear or non-linear coupling boundary conditions are imposed.

References:

[1] Heimann, Lehrenfeld, Preuß (2023): *Geometrically Higher Order Unfitted Space-Time Methods for PDEs on Moving Domains*, SIAM J. Sci. Comput. 45 (2) B139-B165.

[2] Heimann, Lehrenfeld (2025): *Geometry error a*nalysis of a parametric mapping for higher order unfitted space–time methods, IMA J. Numer. Anal., drae098.

[3] Heimann, Lehrenfeld, Preuß (2025): *Discretization Error Analysis of a High Order Unfitted Space-Time Method for moving domain problems*, arXiv preprint 2504.08608.

[4] Heimann (2025): *A Higher Order Unfitted Space-Time Finite Element Method for Coupled Surface-Bulk Problems*, in: Springer LNCSE 153, Proceedings of ENUMATH 2023, 425–435.

Free-boundary limits of a model for receptor-ligand interactions on evolving domains

Chandrasekhar Venkataraman *(University of Sussex)* & Amal Alphonss *(WIAS)* & Diogo Caetano *(University of Warwick)* & Charlie Elliott *(University of Warwick)*

We consider coupled bulk-surface reaction-diffusion systems modelling receptor-ligand dynamics on an evolving domain. In biologically relevant regimes, we derive various novel free boundary problems as limits of the model. These limiting free boundary problems may be formulated as Stefan-type problems on an evolving hypersurface. Our results are new even in the setting where there is no domain evolution. The models are of particular relevance to a number of applications in cell biology. Numerical simulations of the model illustrating the convergence towards free-boundary problems will be presented.

Modeling and Simulation of Paper Folding

Andrea Bonito *(Texas A& M University)*

The unfolding of a ladybird's wings, the trapping mechanism used by a flytrap, the design of self-deployable space shades, and the constructions of curved origami are diverse examples where strategically placed material defects are leveraged to generate large and robust deformations.

With these applications in mind, we consider plate models incorporating the possibility of curved folds as the limit of thin three-dimensional hyper-elastic materials with defects. This results in a fourth order geometric partial differential equation for the plate deformations further restricted to be isometries. The latter non convex constraint encodes the plates inability to undergo shear nor stretch and is critical to justify large deformations.

We then propose different discontinuous Galerkin methods for the approximation of the deformations. The isometry constraint is linearized and incorporated within a gradient flow. We show that the sequence of resulting equilibrium deformations converges to a minimizer of the exact energy (and, in particular, to an isometry) as the discretization parameters tend to infinity. This theory does not require additional smoothness on the plate deformations besides having a finite energy.

We explore numerically the capabilities of the proposed algorithm and illustrate its efficiency on relevant examples.

Space-time Control of Stokes Swimmers

Shawn W. Walker *(Louisiana State University)* & Antoine Laurain *(University of Duisburg-Essen)*

We study the control of the position of a self-deforming swimming body within a fluid flow modeled by the (quasi-static) Stokes equations. By modifying its shape, which is the control variable, the swimming body can affect a change in its position. The problem can be viewed as controlling a free boundary, since the position of the center of the swimmer depends implicitly on its shape and on the solution of the Stokes equations.

We start by defining the mathematical model and the objective functional for optimizing swimming speed. Then, we perform a formal sensitivity analysis with respect to the swimmer shape and mention some key points in the derivation. We also provide numerical results, using an unfitted finite element formulation, that validate the model and the sensitivity analysis, as well as depict optimized swimming motions.

A convergent finite element algorithm for flows by powers of the Gaussian curvature

Balázs Kovács *(Paderborn University)* & Tim Binz *(Princeton University)* and Christian Lubich *(University of Tübingen)*

In this talk we will discuss a error estimates for a numerical solution Gaussian curvature flow of surfaces.

We will present the algorithm based on evolving surface finite elements discretising evolution equations for geometric quantities in particular the second fundamental form and normal vector; give insight into the stability estimates, which has surprising connections to perturbation results for eigenvalues and pseudo-inverses; which lead to optimal-order H^1-norm semi-discrete error estimates.

An Energy-stable Numerical Approximation for the Willmore Flow

Yifei Li & Weizhu Bao *(University of Tübingen)*

The Willmore energy has widespread applications in differential geometry, cell membranes, optical lenses, materials science, among others. The Willmore flow, as the L^2 gradient flow dissipating the Willmore energy, serves as a fundamental tool for its analysis. Despite its importance, the development of energy-stable parametric methods for the Willmore flow remains open. In this talk, I will present a novel energy-stable numerical approximation for the Willmore flow. I begin by introducing our method for planar curves, then demonstrating the underlying ideas – the new transport equation and the time derivative of the mean curvature, that ensure energy stability. Finally, we discuss the extension of our approach to surfaces in 3D.

Elastic Flow Revisited

Paola Pozzi & Björn Stinner *(University of Duisburg-Essen)*

The elastic flow for curves is one of the most important examples of fourth order geometric flows and it has been extensively studied in the past years. From a numerical point of view it is well known that detrimental grid deformations might occur as the curve undergoes strong deformations. In this talk I will revisit the definition of elastic flow and propose an alternative formulation whose FEM discretization provides good grid properties while being amenable for error analysis. I will address some analytical aspects of the flow and then focus on the error analysis of the numerical scheme.

Stability of an ALE method for fluid-structure interactions

Bangwei She *(Capital Normal University)*

When the boundary of a fluid domain consists of a

thin structure, such as deformable plates or shells, the fluid stress exerted on the structure induces its motion, leading to a time-dependent fluid domain. In this scenario, we must not only account for the force interactions between the fluid and the thin structure but also address the velocity field coupling at their interface, which poses significant challenges for numerical simulations. In this paper, we employ the Arbitrary Lagrangian-Eulerian (ALE) method to investigate the stability of numerical solutions for coupled systems involving viscous fluids and thin-walled structures.

Dynamic Ritz projection of finite element methods for fluid-structure interaction

Rong Tang & Erik Burman & Buyang Li *(The Hong Kong Polytechnic University)*

Regardless of the development of various finite element methods for fluid-structure interaction (FSI) problems, optimal-order convergence of finite element discretizations of the FSI problems in the $L^\infty(0,T;L^2)$ norm has not been proved due to the incompatibility between standard Ritz projections and the interface conditions in the FSI problems. To address this issue, we define a dynamic Ritz projection (which satisfies a dynamic interface condition) associated to the FSI problem and study its approximation properties in the $L^\infty(0,T;H^1)$ and $L^\infty(0,T;L^2)$ norms. Existence and uniqueness of the dynamic Ritz projection of the solution, as well as estimates of the error between the solution and its dynamic Ritz projection, are established. By utilizing the established results, we prove optimal-order convergence of finite element methods for the FSI problem in the $L^\infty(0,T;L^2)$ norm.

Convergence of finite element methods for Ricci flow

Guangwei Gao *(The Hong Kong Polytechnic University)* & Evan S. Gawlik *(Santa Clara University)* & Buyang Li *(The Hong Kong Polytechnic University)*

The convergence of a finite element discretization for the two-dimensional Ricci flow is proved. In this method, the Ricci flow on a two-dimensional surface is formulated into solution-driven metric evolution, with metric evolution driven by the Gauss curvature which satisfies a parabolic equation that in turn depends on the metric, thereby enhancing the parabolic structure of the problem. The solution-driven metric evolution formulation is discretized by the finite element method, and the convergence of finite element approximations is proved by adapting the matrix-vector formulation developed in the literature initially for studying solution-driven surface evolution in extrinsic curvature flow. In addition to its convergence, the proposed method also preserves important geometric structures of the Ricci flow at the discrete level, such as area conservation, the Gauss-Bonnet theorem, and the asymptotic behavior of curvature. Extensive numerical experiments are presented to demonstrate the convergence of the proposed method as well as the simulation of Ricci flow.

Error analysis of a finite element scheme for rough PDEs on evolving curves

Björn Stinner (*University of Warwick*) & Paola Pozzi (*Universität Duisburg-Essen*)

Inspired by applications in cell biology we study parabolic partial differential equations on evolving curves with noisy source or reaction terms. We specifically have stochastic approaches to the 'rough' components in mind. Solutions typically lack regularity that is required to show optimal convergence rates of established numerical methods, specifically with respect to the dependence on time. We present a novel scheme based on a suitable time-integrated variational version of the stochastic PDE, which uses linear surface finite elements and a semi-implicit time discretisation. Convergence in mean is proved where the rates depend on the regularity of the solution. We also discuss some numerical simulations that underpin the theoretical findings.

Minisymposium M2

Advances on nonstandard Galerkin methods - part 1

Organiser
Zhaonan Dong

A new control volume method for linear elasticity on quadrilateral grids

Lina Zhao & Shubin Fu *(City University of Hong Kong)*

In this talk, I will present a novel control volume method that is locally conservative and locking-free for linear elasticity problem on quadrilateral grids. The symmetry of stress is weakly imposed through the introduction of a Lagrange multiplier. As such, the method involves three unknowns: stress, displacement and rotation. To ensure the well-posedness of the scheme, a pair of carefully defined finite element spaces is used for the stress, displacement and rotation such that the inf-sup condition holds. An appealing

feature of the method is that piecewise constant functions are used for the approximations of stress, displacement and rotation, which greatly simplifies the implementation. In particular, the stress space is defined delicately such that the stress bilinear form is localized around each vertex, which allows for the local elimination of the stress, resulting in a cell-centered system. The convergence analysis will be shown for the scheme. Several numerical experiments will be performed to verify the performance of the proposed scheme.

Virtual element methods for a class of fully nonlinear elliptic PDEs

Guillaume Bonnet & **Andrea Cangiani** (*SISSA*) & Andreas Dedner & Ricardo H. Nochetto

We develop and analyze a class of H^2-conforming Virtual Element Methods (VEM) for approximating strong solutions to fully nonlinear second-order elliptic partial differential equations of Isaacs type. These problems arise in the context of stochastic differential games and are characterized by their non-divergence form and inherent nonlinearity. Under a structural Cordes condition on the coefficients and of convexity on the domain, we reformulate the continuous problem into a well-posed variational formulation for which we propose a discretisation based on the H^2-conforming Virtual Element Method (VEM). We establish well-posedness via monotonicity arguments based on Miranda–Talenti-type inequalities and prove rigorous a priori error estimates. Numerical experiments are outlined to support the theoretical findings and assess the practical performance of the scheme.

Finite element methods for parametric PDEs

Andreas Rupp & Jay Gopalakrishnan & Vesa Kaarnioja *(Saarland University)*

We derive parametric regularity bounds for a balance equation of the form $\nabla \cdot \mathbf{q} = f$, where $\mathbf{q}$ represents the flux of an unknown quantity u, under abstract assumptions on a random parameter a that links $\mathbf{q}$ and u. A prime example where our theory applies is the diffusion equation, where the parameter a corresponds to the inverse of the diffusivity, i.e., $\mathbf{q} = -a^{-1}\nabla u$. The parameter a is modeled as a Gevrey-regular random field; specifically, we consider random fields that can be expressed as functions of countably infinite sequences of independent random variables, which may be uniformly or normally distributed. We then derive quasi-Monte Carlo (QMC) error bounds for these problems and observe that our QMC method converges optimally if the quantity of interest continuously depends on the unknown function u, its flux $\mathbf{q}$, or its gradient ∇u.

Our analysis encompasses a broad class of balance equations discretized by various finite element methods, provided they satisfy our abstract assumptions. In particular, we demonstrate that these assumptions hold for the diffusion equation discretized using conforming finite elements, mixed methods, and hybridizable discontinuous Galerkin schemes.

Numerical experiments confirm our analytical findings, highlighting the crucial role of the flux in QMC methods. Since all other quantities rely on its optimal convergence and continuous dependence, accurate flux approximation is key to achieving optimal convergence rates.

Adaptive mesh strategies to speed up flow simulations in large-scale fractured media

Zhaonan Dong & Alexandre Ern & Florent Hédin & **Géraldine Pichot** *(Inria Paris & ENPC)* & Nicolas Pignet

In underground environments, fractures are numerous and present at all scales (from cm to km), with very heterogeneous properties. The most commonly used model for fractured rocks is the Discrete Fracture Matrix (DFM) model, in which fractures are represented as structures of codimension 1 (Discrete Fracture Network - DFN). In this work, stochastic DFNs are generated with the software DFN.lab. It enables the generation of cubic-meter fractured rocks, containing over one million of fractures. The objective is to simulate flow in such large-scale fractured media. The challenge is that classical mesh generation with simplices generates several millions of elements. The computational costs of flow simulations could therefore be prohibitive. To save computational time and resources, mesh agglomeration strategies that create polygonal/polyhedral meshes from simplicial meshes are very promising. But they require two main ingredients: discretization methods capable of supporting general elements and a posteriori error estimates to drive the mesh agglomeration. As discretization methods, we focus on the Hybrid High-Order (HHO) methods. HHO methods handle generally shaped elements (polygonal and polyhedral) and produce high-order, optimally converging, and locally conservative discrete solutions. For the a posteriori error estimates, we propose to use recently derived residual-type estimators for HHO methods on elliptic problems, which are robust with respect to the number and measure of faces per element. Several benchmark test cases are presented to illustrate how adaptive mesh strategies combined with HHO methods reduce the number of unknowns without compromising the accuracy of flow

simulations in large-scale DFNs.

Nonconforming virtual element method for the fully nonlinear Monge-Ampère equation

Scott Congreve, Alice Hodson, & Anwesh Pradhan *(Charles University)*

The Monge-Ampère equation is a well known example of a fully nonlinear second-order partial differential equation. By use of the vanishing moment method, it is possible to approximate the solution as a fourth-order quasilinear partial differential equation. In this talk, we consider a C^1-nonconforming virtual element method (VEM) approximation of this quasilinear PDE that is C^0-conforming. We show the uniqueness and existence of the solution of this approximation, and derive a priori error estimates which are comparable with existing methods (such as the finite element method for the vanishing moment problem).

A hybrid high-order method for the biharmonic problem

Ngoc Tien Tran & Yizhou Liang *(Universität Augsburg)*

This talk proposes a new hybrid high-order discretization for the biharmonic and the corresponding eigenvalue problems. The discrete ansatz space includes degrees of freedom in $n-2$ dimensional submanifolds in addition to the typical degrees in the mesh and on the hyperfaces in the literature, e.g., nodal values in 2d and edge values in 3d. This allows for the characteristic commuting property in the hybrid high-order methodology in any space dimension and, consequently, lower eigenvalue bounds of higher order for the eigenvalue problem. The main results are a priori and a posteriori error estimates. The latter motivates an adaptive mesh refining algorithm that empirically recovers optimal convergence rates for singular solutions.

An asymptotically hypocoercive space-time discontinuous Galerkin method for the Kolmogorov equation

Philip J. Herbert *(University of Sussex)*, Zhaonan Dong *(Inria, CERMICS)*, & Emmanuil H. Georgoulis *(Heriot-Watt, NTU Athens, IACM-FORTH)*

The study of kinetic equations, it is sometime the case that one has a degenerate evolution problems have the property that diffusion exists in only *some* directions. Despite this property, they may exhibit convergence to equilibrium over a long time period. These equations may arise as a Fokker–Planck equation which describes the time evolution of the probability density function of a stochastic processes. In this talk we will describe and analyse a fully discrete scheme for the Kolmogorov equation in a finite domain using a discontinuous Galerkin discretisation. We will demonstrate that the formulation we describe has estimates which are robust with respect to final time, demonstrating some form of decay to equilibrium.

Vortex-capturing multiscale spaces for the Ginzburg-Landau model of superconductivity

Christian Döding *(University of Bonn)* & Maria Blum & Benjamin Dörich & Patrick Henning

Superconductors subjected to magnetic fields exhibit rich and intricate phenomena, such as the formation of so-called Abrikosov vortex lattices. These patterns arise as minimizers of the Ginzburg-Landau energy, but their accurate numerical approximation remains challenging due to the need for fine mesh resolutions. In this talk, we present a novel approach based on Localized Orthogonal Decomposition—a multiscale method that constructs problem-adapted approximation spaces. Applied to the Ginzburg-Landau model, this technique yields a high-order method under mild regularity assumptions and significantly relaxes the resolution condition of traditional finite element methods. As a result, it enables the accurate approximation of vortex structures even on coarse computational grids with only a few degrees of freedom.

Data-dependent density estimation for the Fokker-Planck equation in higher dimensions

Max Jensen & Fabian Merle, Andreas Prohl *(University College London)*

We present a new strategy to approximate the global solution of the Fokker-Planck equation efficiently in higher dimensions and show its convergence. The main ingredients are the Euler scheme to solve the associated stochastic differential equation and a histogram method for tree-structured density estimation on a data-dependent partitioning of the state space R^d.

Minisymposium M3

Advances on nonstandard Galerkin methods - part 2
Organiser
Lorenzo Mascotto

On the VEMs and IFEMs: spaces, complexes and the applications to electromagnetic interface problems

Ruchi Guo *(Sichuan University)* & Shuhao Cao *(University of Missouri–Kansas City)*

Electromagnetic interface problems widely appear in a lot of engineering applications, such as electric actuators, invasive detection techniques and integrated circuit, which are typically described by Maxwell equations with discontinuous coefficients. Conventional finite element methods require a body-fitted mesh to solve interface problems, but generating a high-quality mesh for complex interface geometry is usually very expensive. Instead, using unfitted mesh finite element methods can circumvent mesh generation procedure, which greatly improves the computational efficiency. However, the low regularity of Maxwell equations makes its computation very sensitive to the conformity of the approximation spaces. This very property poses challenges on unfitted mesh finite element methods, as most of them resort to non-conforming spaces. In this talk, we will present our recent progress including several methods for this topic.

How far are two symmetric matrices from commuting? With an application to object characterisation and identification using *hp*-FEM in metal detection

P.D. Ledger, W.R.B. Lionheart & J. Elgy *(University of Leicester)*

In metal detection, eddy currents are induced in highly conducting objects by low-frequency time varying magnetic fields and inductive measurements are made. Metal detection has applications including security screening, locating antipersonnel landmines, identifying foreign objects for food safety, scrap sorting, archaeology and treasure hunting. The magnetic field perturbation in the eddy current case can be described by an asymptotic expansion as the object size tends to zero. Here, the leading order term object provides object characterisation information through a polarizability tensor description whose coefficients are a function of the exciting frequency, the object's shape and its materials. The leading order term in the expansion can be simplified so that it can be expressed in terms of a rank two complex symmetric magnetic polarizability tensor (MPT), which reduces the number of coefficients required for the description. So that the MPT offers an economical characterisation of conducting magnetic objects, which can be obtained from measurements of the induced voltage.

The MPT characterisation can be computed for known objects that one might encounter in a detection scenario and we review algorithms for efficiently and accurately computing the MPT coefficients using *hp*-finite element analysis and discretisations based on unstructured meshes with prismatic boundary layers and high order $\mathbf{H}(\mathrm{curl})$ conforming elements. We will also review an adaptive proper orthogonal decomposition reduced order model to efficiently compute the MPT spectral signature (MPT coefficients as a function of frequency) to provide additional characterisation information. To improve the machine learning (ML) classification of an object from the MPT spectral signature, we have previously used a dataset of a large number of objects and eigenvalues/ tensor invariants of the real and imaginary parts of the complex symmetric rank two MPT, sampled at discrete frequencies, as features. In this talk, our interest in this work focuses on examining whether rotational information obtained from the real and imaginary parts of the MPT spectral signature could add further feature information to assist with the classification.

Traditionally Riemannian and Euclidean metrics are applied to examine the extent to which measurements of rotation matrices are close to each other. However, when rotational matrices are obtained from eigenvectors of measured symmetric matrices, this can be problematic if the associated eigenvalues are close. In this talk, we present novel semi-metrics that can be used to approximate the Riemannian metric for small angles. Our new results do not require eigenvector information and are beneficial for measured datasets. There are also issues when using comparing rotational data arising from computational simulations and it is important that the impact of the approximations on the computed outputs is properly assessed to ensure that the approximations made and the finite precision arithmetic are not unduly polluting the results. We will present an analysis which demonstrates that using an appropriate *hp*-finite element discretisation to compute the MPT spectral signature achieves this. We also describe how our new approximate measures of distance provide additional feature information, which is invariant of the object orientation, to aid with ob-

ject identification using ML classifiers.

A Positivity-Preserving Finite Element Framework for Accurate Dose Computation in Proton Therapy

Tristan Pryer & Ben S. Ashby & Abdalaziz Hamdan *(University of Bath)*

We present a stabilised finite element method for modelling proton transport in tissue, incorporating both inelastic energy loss and elastic angular scattering. A key innovation is a positivity-preserving formulation that guarantees non-negative fluence and dose, even on coarse meshes. This enables reliable computation of clinically relevant quantities for treatment planning. We derive a priori error estimates demonstrating optimal convergence rates and validate the method through numerical benchmarks. The proposed framework provides a robust, accurate and efficient tool for advancing proton beam therapy.

Equivalence of mixed and nonconforming polytopal methods

Simon Lemaire *(INRIA, University of Lille)*

Since the seminal papers by Arnold & Brezzi (1985) and Arbogast & Chen (1995), it is well understood, in the finite element context, and for diffusion problems, that (conforming) mixed methods can be equivalently recast into (primal) nonconforming methods, providing a very handy and efficient way of implementing mixed methods. The most famous example in this respect is perhaps the equivalence, on simplices, between the lowest-order (mixed) Raviart–Thomas method and a bubble-enriched version of the (primal) Crouzeix–Raviart method (up to a slight modification of its right-hand side). For higher polynomial degrees, the resulting primal (nonconforming) schemes take the form of what Arbogast & Chen term projection methods. The objective of this talk is to discuss similar questions in the context of polytopal methods.

A cut finite element method for problems in evolving domains

Sara Zahedi & Sebastian Myrbäck *(KTH Royal Institute of Technology, Sweden)*

In this talk, I will introduce a Cut Finite Element Method (CutFEM) for convection-diffusion equations in time-dependent domains. The method relies on an unfitted space-time discretization that employs quadrature rules in time and stabilization techniques to avoid the explicit construction of space-time meshes. I will discuss high-order discretizations and demonstrate how global mass conservation is achieved by applying Reynolds' transport theorem. Numerical examples will be presented for both bulk problems and coupled bulk-surface systems.

Nodally bound-preserving composite discontinuous Galerkin methods

Emmanuil H. Georgoulis *(Heriot-Watt University & NTU Athens)* & Abdoreza Amiri *(University of Strathclyde)* & Gabriel R. Barrenechea *(University of Strathclyde)* & Tristan Pryer *(University of Bath)*

We will introduce a nonlinear discontinuous Galerkin method on general polygonal/polyhedral elements, with user-selected nodal values within each polygon/polyhedron preserving bounds known for the exact solution, e.g., positivity or a maximum global value. The method is *composite* in the sense that each polygonal/polyhedral element is further subdivided into simplices, whose nodal values are preserved. Crucially, the computational complexity of the method is that of the "coarse" polygonal/polyhedral mesh and *not* of the simplicial subdivision. The discrete problem involves a nonlinear projection operator mapping arbitrary nodal values within each polygonal/polyhedral element into bound-preserving ones and seeks the numerical solution in the range of this projection. To ensure injectivity, a stabilisation is introduced, possessing a key monotonicity property. A salient feature of the proposed method is that it accepts arbitrary number of user-selected bound-preserving nodal values per element. We will present *a priori* error analysis for the case of the discontinuous Galerkin method applied to elliptic PDEs and discuss the intricacies of the construction of bound-preserving interplants. Numerical experiments showcasing the practicality of the method will be given.

Unfitted finite element methods for the biharmonic and Cahn-Hilliard problem in primal form

André Massing *(Norwegian University of Science and Technology)* & Isak Hammer & Eric Neiva (CNRS, Collège de France)

In this talk, we present unfitted finite element methods for the numerical solution of the biharmonic and Cahn-Hilliard equation on embedded (or potentially moving) domains. Our approach combines the continuous interior penalty method from [1] with the unfitted finite element techniques introduced in [2, 3] to devise geometrically robust schemes for the pri-

mal 4th-order Cahn-Hilliard formulation. As a consequence, we are able to derive stability, a priori error, and condition error estimates for the linearized biharmonic equation with Cahn-Hilliard type boundary conditions resembling the classical results from [1] obtained on conform meshes. The theoretical estimates hold for order $p \geq 2$. Afterwards, we demonstrate how the resulting spatial discretization scheme can be combined with first and second-order BDF-based timestepping methods to numerically solve the complete Cahn-Hilliard equation on domains which are embedded into a structured background mesh. Finally, we provide ample numerical results to corroborate our theoretical findings and discuss possible advantages and disadvantages of the presented formulations.

References

[1] S. C. Brenner, S. Gu, T. Gudi, and L. Sung. A quadratic C^0 interior penalty method for linear fourth order boundary value problems with boundary conditions of the Cahn–Hilliard type. *Int. J. Numer. Meth. Engng.*, Vol. **50**(4), pp. 2088–2110, 2012.

[2] E. Burman, S. Claus, P. Hansbo, M. G. Larson, and A. Massing. CutFEM: discretizing geometry and partial differential equations. *SIAM J. Numer. Anal.*, Vol. **104**, pp. 472–501, 2015.

[3] S. Badia, F. Verdugo, and A.F. Martín, Alberto F. The Aggregated Unfitted Finite Element Method for Elliptic Problems. *Comput. Methods Appl. Mech. Engrg.*, Vol. **336**, pp. 533–553, 2018.

The Bound Preserving Method Applied to the 2D Induction Heating Problem.

Katherine MacKenzie & Gabriel Barrenechea *University of Strathclyde*

Induction heating is a process widely used in the metallurgical manufacturing industry to heat conductive materials. Using an alternating current with a very high frequency, a magnetic field generates a current in the material, which produces heat due to the Joule heating process. This current is concentrated in a very thin layer near the boundary of the material, and as such there is a boundary layer in the magnetic field. This creates what appears to a highly irregular source term ($f \in L^1(\Omega)$), which can cause difficulties when proving well-posedness. However, by adapting arguments used for the (simpler) Thermistor problem [1], we can prove an existence and regularity result for the weak solution, and thus circumvent the main challenges that would arise due to an irregular right-hand side.

In this talk, we will describe the application of the Nodally Bound Preserving Method [2] to the Induction Heating problem. This method is designed to satisfy given bounds on the solution and guarantees stability for meshes for which standard methods don't guarantee bound preservation. The main technical aspect is to show that, when imposing non-physical bounds on the discrete solution, the method converges to the best approximation in the infinite-dimensional constrained convex set. As a result, for the induction heating problem, where the bounds are not explicit, this leads to a method that converges without imposing a restriction on the mesh.

References

[1] M. J. Holst, M. G. Larson, A. Målqvist and R. Söderland. "Convergence analysis of finite element approximations of the Joule Heating problem in three spatial dimensions." BIT Numer Math 50 (2010) 781-795

[2] G. R. Barrenechea, E. H. Georgoulis, T. Pryer, and A. Veeser. "A Nodally Bound-Preserving Finite Element Method." IMA journal of numerical analysis 44.4 (2024): 2198–2219

hp-Version discontinuous Galerkin methods for the *p*-Laplacian

Panagiotis Paraschis & Konstantinos Chrysafinos, Emmanuil H. Georgoulis *(National Technical University of Athens)*

We consider the full discretization of the elliptic and parabolic p-Laplacian with discontinuous Galerkin methods. Stability and quasi-norm error estimates are being considered for the discontinuous-in-time Galrekin method with conforming finite elements in space. We also consider an hp-version discontinuous Galerkin method for the elliptic p-Laplacian and a space-time discontinuous Galerkin method for the underlying parabolic problem, in polygonal curved meshes. With the help of new quasi-norm trace-inverse estimates, we derive stability and quasi-norm error bounds of optimal order with respect to the mesh size and slightly suboptimal order with respect to the local

polynomial degrees.

Minisymposium M4

Numerical methods for Mean Field Games
Organisers
Yohance Osborne, Iain Smears and Harry Wells

A high-order scheme for mean field games

Elisa Calzola & Elisabetta Carlini & Francisco J. Silva *(University of Verona)*

We propose a high-order numerical scheme for time-dependent mean field games systems. The scheme, which is built by combining Lagrange–Galerkin and semi-Lagrangian techniques, is consistent and stable for large time steps compared with the space steps. We provide a convergence analysis for the exactly integrated Lagrange–Galerkin scheme applied to the Fokker–Planck equation, and we propose an implementable version with inexact integration. Finally, we validate the convergence rate of the proposed scheme through the numerical approximation of two mean field games systems.

A posteriori error bounds for finite element approximations of steady-state mean field games

Harry Wells *(University College London)*

In this talk, we present the derivation and analysis of *a posteriori* error bounds for stabilized finite element discretizations of second-order stationary mean field games [1]. A key motivation for *a posteriori* analysis is that it produces computable error estimators, based solely on the numerical solution, which provide rigorous bounds on the approximation error. These estimators can also be used in adaptive algorithms to improve accuracy in a systematic and efficient way.

We begin by proving an equivalence, at the continuous level, between the H^1-norm of the error and the dual norms of the residuals associated with the underlying Hamilton–Jacobi–Bellman and Kolmogorov–Fokker–Planck equations. This result forms the basis for deriving reliable and efficient error estimators for a broad class of stabilized first-order finite element methods. The estimators consist of standard residual-type terms, commonly found in the literature, along with additional contributions from the stabilization.

We then show that under more restrictive assumptions on the stabilization method, in particular the restriction to *patchwise affine preserving* stabilizations, we can derive an improved estimator that is independent of the specific stabilization method used. The benefits of these restrictions in stabilization techniques include localisability, simpler implementation and computation, and utilization of the estimator in adaptive mesh refinement algorithms. This result also contributes to the wider analysis of error estimation for stabilized finite element methods.

We conclude with numerical experiments that support the theoretical results and demonstrate the performance of the proposed estimators on challenging problems without known analytical solutions. Additionally, we showcase adaptive finite element methods that improve computational efficiency and accuracy for mean field games posed on nonconvex domains with low-regularity solutions.

This is joint work with Yohance A. P. Osborne (*Durham University*) and Iain Smears (*University College London*).

References

[1] Yohance A. P. Osborne, Iain Smears, and Harry Wells. A posteriori error bounds for finite element approximations of steady-state mean field games. *arXiv preprint arXiv:2502.14687*, 2025.

Numerical Approximations of Newton algorithm for Mean Field Games

Elisabetta Carlini *(Sapienza University of Rome)*, F.J. Silva & A. Zorkot

We propose two numerical approximations for second-order Mean Field Games (MFG) systems, based on the discretization of the Newton algorithm for MFG systems recently introduced by F. Camilli and Q. Tang (2023).

The proposed methods rely on a semi-Lagrangian scheme and a finite-difference scheme. We compare them with Newton's finite-dimensional method applied to the discrete finite-difference system introduced by Y. Achdou and I. Capuzzo Dolcetta (2010).

Nearly and Fully Quasi-optimal Finite Element Approximations of Second-order Mean Field Game Systems

Yohance Osborne *(University of Durham)*

We present error bounds for monotone stabilized finite element discretizations of stationary second-order

mean field games (MFG) on Lipschitz polytopal domains. Under suitable hypotheses, we prove that the approximation is asymptotically nearly quasi-optimal in the H^1-norm in the sense that, on sufficiently fine meshes, the error between the exact and computed solutions is bounded by the best approximation error of the corresponding finite element space, plus possibly an additional term, due to the stabilization that is of optimal order with respect to the mesh size. We thereby deduce optimal rates of convergence of the error for sufficiently regular solutions, as well as full asymptotic quasi-optimality of the error in the more restricted case of sequences of strictly acute meshes. When the domain is convex, we show that the convergence rate for the H^1-norm error of the value function approximation remains optimal even if the density function only has minimal regularity in H^1.

Monotonicity-based methods for mean-field games

Diogo Gomes & Rita Ferreira & Melih Ucer *(King Abdullah University of Science and Technology)*

This presentation explores mean field games (MFGs) through the lens of functional analysis, focusing on the role of monotonicity methods in understanding their properties and deriving solutions. Monotonicity operators emerge as a central tool in our analysis. We establish the connection between monotone operators and variational inequalities, showcasing how the latter offers a flexible framework for addressing situations where traditional solutions may not exist. Building on this foundation, we extend our discussion to the Banach space setting, examining monotone operators between a Banach space and its dual. We present existence theorems and regularization methods tailored to this context. We conclude by exploring the concept of weak-strong uniqueness, which establishes conditions under which weak and strong solutions of MFGs coincide.

A network model for urban planning

Adriano Festa & Fabio Camilli & Luciano Marzufero *(Politecnico di Torino)*

We study a mathematical model to describe the evolution of a city, which is determined by the interaction of two large populations of agents, workers and firms. The map of the city is described by a network with the edges representing at the same time residential areas and communication routes. The two populations compete for space while interacting through the labour market. The resulting model is described by a two population Mean-Field Game system coupled with an Optimal Transport problem. We prove existence and uniqueness of the solution and we provide several numerical simulations.

Minisymposium M5

Interplay of solvers, discretisations and geometries in the numerical approximation of eigenvalue problems

Organisers
Fleurianne Bertrand and Philipp Zilk

Approximation of parametric eigenvalues – with applications to interior transmission eigenvalue problems

Davide Pradovera & Alessandro Borghi & Andreas Kleefeld & Lukas Pieronek *(KTH Royal Institute of Technology)*

PDE-based eigenvalue problems are of interest in many applications, e.g., in the analysis of time-harmonic mechanical vibrations or wave propagation. Parameters are often included in the eigenvalue problem, as a way to model uncertainties or design variables. In this context, we propose a strategy for solving the "forward problem": parametric (nonlinear) eigenproblems.

For a wider applicability of our method, we stay non-intrusive: we make no assumptions on how the problem depends on the eigenvalue or on the parameters. Our method piggybacks on a reliable contour-integration-based eigensolver for dealing with non-parametric versions of the target problem, obtained by "freezing" the parameters at some collocation parameter values. Then the collection of obtained eigenvalues is used to synthesize the eigenvalue manifolds, i.e., to understand how the eigenvalues vary as the parameters change.

Several issues arise, mostly due to the possible irregularity in the eigenvalue manifolds: (i) manifold crossings may happen if the target spectrum is not well isolated, (ii) bifurcations may reduce the smoothness of the manifolds, and (iii) the target manifolds may "appear and disappear" as parameters vary, since eigenvalues may migrate outside the integration contour. We describe a strategy to flag these undesirable effects, and, to some extent, to circumvent them.

To showcase the effectiveness of our approach, we present some ongoing work on *interior transmission*

eigenvalue problems

$$\begin{cases} -\Delta v = \lambda^2 v & \text{in } D, \\ -\Delta w = (\lambda n)^2 w & \text{in } D, \\ v = w & \text{on } \partial D, \\ \partial_\nu v = \partial_\nu w & \text{on } \partial D. \end{cases}$$

These are of interest in inverse problems involving the Helmholtz equation, where the value of the refraction index n must be inferred from spectral data. Despite the purely real nature of the PDE-based problem, complex eigenvalues arise for almost all values of the parameter n. We describe theoretical results and empirical evidence showing that such complex eigenvalues may display bifurcations.

Mixed finite element for Stokes eigenvalue problem

Tugay Dagli & Fleurianne Bertrand *(TU Chemnitz)*

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 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 Raviart-Thomas space for the stress, the space of discontinuous piecewise vectors for the velocity, and the space of continuous piecewise functions 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 $k \geq 1,\ d = 2, 3$. 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.

Detecting Near Resonances Using Randomized Hierarchical Matrix Factorizations

Luka Grubišić & Ralf Hiptmair & Luka Marohnić *(University of Zagreb)*

In this talk, we investigate the Helmholtz transmission problem. Our primary focus is on identifying the values of the spectral parameter which lead to near-resonant behavior (local extrema of the resolvent norm). To address this task numerically, we utilize a randomized singular value decomposition (SVD) tailored to the structure of the stiffness matrix of the Galerkin discretization of the boundary integral operators. We use hierarchical matrix factorizations, such as hierarchical LU factorization of Hackbusch et al., to speed up the sampling of the resolvent. The search of the extrema is based on the surrogate modelling of the dependence of the norm of the resolvent on the spectral parameter.

A complex-projected Rayleigh quotient iteration for targeting interior eigenvalues

Nils Friess & Alexander D. Gilbert & Robert Scheichl *(Universität Heidelberg)*

We introduce a new *projected Rayleigh quotient iteration* aimed at improving the convergence behaviour of classic Rayleigh quotient iteration (RQI) by incorporating approximate information about the target eigenvector at each step. While classic RQI exhibits local cubic convergence for Hermitian matrices, its global behaviour can be unpredictable, whereby it may converge to an eigenvalue far away from the target, even when started with accurate initial conditions. The key idea of the new algorithm is at each step to add a complex-valued projection to the original matrix (that depends on the current eigenvector approximation), such that the unwanted eigenvalues are lifted into the complex plane while the target stays close to the real line, thereby increasing the spacing between the target eigenvalue and the rest of the spectrum. Making better use of the eigenvector approximation leads to more robust convergence behaviour and the new method converges reliably to the correct target eigenpair for a significantly wider range of initial vectors than does classic RQI. We show that the new method retains local cubic convergence and present several numerical examples demonstrating its improved global convergence behaviour. In particular, we apply it to compute eigenvalues in a band-gap spectrum of a Sturm-Liouville operator where the target and unwanted eigenvalues are closely spaced.

On the behavior of discrete eigenvalues for lumped mass approximations on trimmed geometries

Yannis Voet & Ivan Bioli *(École Polytechnique Fédérale de Lausanne)*

In structural dynamics, mass lumping techniques are commonly employed for improving the efficiency of explicit time integration schemes and increasing their critical time step constrained by the largest discrete eigenvalue of the system. For immersogeometric methods, Leidinger [1] first showed in 2020 that for sufficiently smooth spline discretizations, the largest eigenvalue was not affected by small trimmed elements if the mass matrix was lumped. Despite compelling nu-

merical evidence, rigorous theoretical explanations are still lacking. This talk unravels the phenomenon. By combining linear algebra with functional analysis, we derive sharp analytical estimates capturing the behavior of the largest discrete eigenvalue for lumped mass approximations and various trimming configurations, covering both 1D and 2D problems. Our results confirm the prominent role smoothness plays in ensuring that the largest eigenvalue remains bounded. However, there is another side to the story. While the largest eigenvalues may remain bounded, the smallest ones instead converge to zero, thereby introducing spurious eigenvalues and modes in the low-frequency spectrum. If activated, those modes may disastrously impact the solution, as recently shown in [2].

References

[1] L. Leidinger, Explicit Isogeometric B-Rep Analysis for Nonlinear Dynamic Crash Simulations, Ph.D. thesis, Technische Universität München (2020).

[2] Y. Voet, E. Sande, A. Buffa, Mass lumping and stabilization for immersogeometric analysis, arXiv preprint arXiv:2502.00452 (2025).

The Isospectral Problem for Cracks in Membranes: Perspectives from Spectral Geometry and Numerical Simulation

Philipp Zilk & Thomas Apel *(Universität der Bundeswehr München)*

The Laplace spectrum of a domain encodes fundamental geometric information, including the presence of singularities. The inverse spectral problem – whether one can "hear" the shape of a domain – was popularized by Kac in 1966 and has since been extensively studied. We investigate this problem in the context of cracks, examining their spectral imprint and the extent to which they can be detected from eigenfrequencies.

We first present an analytical approach based on the short-time asymptotic expansion of the heat trace, a well-known spectral invariant. By synthesizing and extending existing results, we establish explicit connections between cracks and the corresponding eigenfrequencies of the domain. To complement this analysis, we introduce a data-driven approach based on simulated spectral data to detect the presence of cracks and identify associated geometry parameters. The data is generated using isogeometric analysis, a numerical method known for its excellent spectral approximation properties. Since eigenfunctions associated with corner singularities exhibit reduced regularity, their eigenvalues cannot be reliably approximated using standard methods. To address this, we employ a local refinement strategy based on a singular isogeometric mapping, achieving optimal convergence rates for both eigenfunctions and eigenvalues.

Minisymposium M6

High-order and hp- numerical methods for PDEs

Organiser
Scott Congreve

***hp*-error analysis of mixed-order hybrid high-order methods for elliptic problems on simplicial meshes**

Zhaonan Dong & Alexandre Ern *(INRIA Paris & ENPC)*

We present both *hp*-a priori and *hp*-a posteriori error analysis of a mixed-order hybrid high-order (HHO) method to approximate second-order elliptic problems on simplicial meshes. Our main result on the *hp*-a priori error analysis is a $\frac{1}{2}$-order p-suboptimal error estimate. This result is, to our knowledge, the first of this kind for hybrid nonconforming methods and matches the state-of-the-art for other nonconforming methods as discontinuous Galerkin methods. Our second main result is a residual-based *hp*-a posteriori upper error bound, comprising residual, normal flux jump, tangential jump, and stabilization estimators (plus data oscillation terms). The first three terms are p-optimal and only the latter is $\frac{1}{2}$-order p-suboptimal. This result is, to our knowledge, the first *hp*-a posteriori error estimate for HHO methods. A novel approach based on the partition-of-unity provided by hat basis functions and on local Helmholtz decompositions on vertex stars is devised to estimate the nonconformity error. Finally, we establish local lower error bounds. Remarkably, the normal flux jump estimator is only $\frac{1}{2}$-order p-suboptimal, as it can be bounded by the stabilization owing to the local conservation property of HHO methods. Numerical examples illustrate the theory.

A posteriori error estimates of a DG-CG method for the wave equation in second order formulation

Lorenzo Mascotto & Zhaoanan Dong, Zuodong Wang *(University of Milano-Bicocca)*

We establish semi-discrete in time a posteriori error estimates for a discontinuous-continuous Galerkin dis-

cretization of the wave equation in second order formulation; the resulting method is a Petrov-Galerkin scheme based on piecewise and piecewise continuous polynomial in time test and trial spaces, respectively. More precisely, we exhibit constant-free, reliable a posteriori error estimates for the error measured in the $L^\infty(L^2)$ norm; to this aim, we design a reconstruction operator into $\mathcal{C}^1$ piecewise polynomials over the time grid with optimal approximation properties in terms of the polynomial degree distribution and the time steps. Numerical examples illustrate the theoretical findings.

New Crouzeix-Raviart elements of even degree and variable order Crouzeix-Raviart spaces

Marialetizia Mosconi & Andrea Bressan & Lorenzo Mascotto *(Università degli Studi di Milano-Bicocca)*

We construct new Crouzeix-Raviart (CR) spaces of even degree p that are spanned by basis functions mimicking those for the standard odd degree case. Compared to the standard even order CR gospel, the present construction allows for the use of nested bases of increasing degree and is particularly suited to design variable order CR methods. We analyze a nonconforming discretization of a two dimensional Poisson problem, which requires a DG-type stabilization. Numerical results are presented, which exhibit the expected convergence rates for the h- and p-versions of the scheme. The design of variable degree CR global spaces and a corresponding method are discussed, along with the assessment of its numerical performance for the approximation of corner singularities using hp-refinements.

High-order robust iterative solvers and optimal complexity of adaptive FEM

Ani Miraçi & Michael Innerberger & Jan Papež & Dirk Praetorius & Julian Streitberger & Martin Vohralík *(TU Wien)*

While standard FEMs rely on underlying uniform meshes, adaptive FEMs (AFEMs), typically encoded in the paradigm SOLVE — ESTIMATE — MARK — REFINE, drive the local mesh refinement to capture potential singularities of the (unknown) PDE solution. Considering a fixed polynomial degree p for the discretization and steered by reliable a posteriori error control, the adaptive algorithm allows to obtain optimal convergence rates with respect to the dimension of the finite element space. Crucially, such rates of convergence are improved by increasing p, hence the importance of high order discretization. However, one should keep in mind that the adaptive algorithm is inherently cumulative in nature: an initial coarse mesh is used as input and exact finite element solutions need to be computed on consecutively refined meshes before a desired accuracy can be ensured. Thus, in practice, one strives instead to achieve optimal complexity, i.e., optimal rate of convergence with respect to the overall computation cost.

The core ingredient needed for optimal complexity consists in the use of appropriate iterative solvers to be integrated as the SOLVE module of the adaptive algorithm. More precisely, one requires: (i) a solver whose iteration step is: (a) of linear complexity and (b) uniformly contractive; (ii) an a-posteriori-steered solver-stopping criterion which allows to discern and balance discretization and solver error; (iii) nested iteration, i.e., the last computed solver-iterate serves as initial guess in the newly-refined mesh.

First, we develop an optimal local multigrid in the context of symmetric linear elliptic second order PDEs and a finite element discretization with a fixed polynomial degree p and a hierarchy of bisection-generated meshes with local mesh size h. The solver contracts the algebraic error h- and p-robustly and comes with a built-in a posteriori estimator equivalent to the algebraic error. Second, the overall adaptive algorithm is then shown to be convergent for any choice of adaptivity parameters (unconditional convergence), and to be of optimal complexity for sufficiently small parameters. Third, we provide extensions to a class of nonlinear PDEs, where a nested iterative solver structure fits into the abstract analytical framework of the linear symmetric case.

Numerical experiments highlight the theoretical results of optimal complexity for adaptivity with iterative solvers and emphasize the practical relevance and gains of such numerical simulations.

Fast solvers for high-order finite element discretizations of the de Rham complex

Charles Parker & Pablo D. Brubeck & Patrick E. Farrell & Robert C. Kirby *(University of Oxford)*

Many applications in electromagnetism, magnetohydrodynamics, and pour media flow are well-posed in spaces from the 3D de Rham complex involving H^1, $H(\mathrm{curl})$, $H(\mathrm{div})$, and L^2. Discretizing these spaces with the usual conforming finite element spaces typically leads to discrete problems that are both structure-preserving and uniformly stable with respect to the mesh size and polynomial degree. Robust preconditioners/solvers usually require the inversion of subproblems or auxiliary problems on vertex, edge, or face patches of elements. For high-order discretizations,

the cost of inverting these patch problems scales like $\mathcal{O}(p^9)$ and is thus prohibitively expensive. We propose a new set of basis functions for each of the spaces in the discrete de Rham complex that reduce the cost of the patch problems to $\mathcal{O}(p^6)$ complexity. By taking advantage of additional properties of the new basis, we propose further computationally cheaper variants of existing preconditioners. Various numerical examples demonstrate the performance of the solvers.

A Pressure-Robust Hybrid High-Order Method for the Unsteady Navier–Stokes Equations

Thomas J. Radley & Lourenço Beirão da Veiga, Daniele A. Di Pietro, Jérôme Droniou, Kirubell B. Haile *(IMAG, Université de Montpellier)*

In recent years, the robustness of classical inf-sup stable mixed discretisations of the Navier–Stokes equations has been studied. Of particular interest is the notion of *pressure-robustness*, which reflects the fact that velocity solutions of the continuous Navier–Stokes problem are unaffected by irrotational body forces. Pressure-robust schemes generate discrete velocities whose errors scale independently of the continuous pressure solution. Many classical mixed methods are not pressure-robust, as they fail to enforce the divergence-free constraint in a pointwise fashion, and thus suffer from pressure-induced locking and suboptimal velocity error estimates.

Schemes for convection-dominated problems may also suffer from non-physical oscillations in the discrete solution. Many stabilisation techniques have been developed to address this issue, but such stabilisations may weaken error estimates through the introduction of inverse powers of the viscosity. Schemes whose velocity error estimates are independent of such terms are referred to as *Reynolds-semi-robust*.

We introduce a pressure-robust and Reynolds-semi-robust scheme employing hybrid velocity and pressure spaces for the incompressible unsteady Navier–Stokes equations. The divergence-free constraint is enforced pointwise through a careful treatment of the velocity–pressure coupling. We prove well-posedness of the scheme and establish a velocity error estimate that is robust with respect to pressure and optimal in the viscous and convective limits. The optimal convergence and pressure-robustness of the scheme will be demonstrated through numerical examples.

An adaptive spectral element method for systems of conservation laws

Manuel Colera–Rico & Vít Dolejší *(Universidad Politécnica de Madrid)*

A novel method for the solution of systems of conservation laws is presented. For the space discretization, the scheme considers high-order continuous finite elements stabilized via subgrid modeling, as well as highly anisotropic adaptive meshes in order to capture any sharp features in the solution with the minimum number of mesh elements. Time integration is carried out via adaptive, linearly implicit formulas, which allow for large time steps and require only the solution of a few linear systems per solved time interval. Numerical experiments, which include a hard case of nonconvex flux and the Euler equations for compressible flows, were performed with up to eight-degree elements and a third-order time marching formula in order to assess the capabilities of the method.

hp-version A priori error estimates of a DG-CG method for the wave equation in second order formulation

Zuodong Wang & Zhaonan Dong, Lorenzo Mascotto *(Ecole Nationale des Ponts et Chaussées, IP Paris; Centre Inria de Paris)*

We establish fully-discrete space-time stability and a priori error estimates for a discontinuous-continuous Galerkin discretization of the wave equation in second order formulation; such estimates are explicit in the spatial mesh size, time steps, and polynomial degrees, and are measured in the $W^{1,\infty}(L^2)$ and $L^\infty(H^1)$ norms. Numerical examples illustrate the theoretical findings.

Iterative *hp*-FEM for semilinear Poisson problems with monomial reaction: Exponential convergence and complexity

Y. He, P. Houston, C. Schwab & **Thomas P. Wihler** *(University of Bern)*

We study the fully explicit numerical approximation of a semilinear elliptic boundary value model problem, which features a monomial reaction and analytic forcing, in a bounded 2d polygon. In particular, we analyse the convergence of *hp*-type iterative linearised Galerkin (*hp*-ILG) solvers. Our convergence analysis is carried out for conforming *hp*-finite element discretisations on sequences of geometric corner meshes, with polynomial degrees increasing in sync with the local mesh refinement. For a sequence of discrete solutions generated by the ILG solver, with a stopping criterion that is consistent with the exponential convergence of the exact *hp*-FE solution, we prove exponential convergence in H^1 to the unique weak solution of the boundary value problem. Numerical experiments illustrate the exponential convergence of the numerical

approximations obtained from the proposed scheme in terms of the number of degrees of freedom as well as of the computational complexity involved.

Minisymposium M7

Recent Advances in Randomised Numerical Linear Algebra

Organisers
Yuji Nakatsukasa and Taejun Park

Performance comparison of randomized Krylov solvers for linear systems

Stefan Güttel & John W. Pearson *(The University of Manchester)*

There are several interesting approaches that aim at speeding up Krylov solvers for large sparse linear systems of equations using randomized sketching. Yet, many challenges remain. These include issues with numerical stability and questions about a fair way to compare these methods against existing solvers. We present a new benchmark collection of challenging systems arising with PDE-constrained optimization. We apply this benchmark to get a better picture of the actual time-to-solution performance of randomized solvers. We also present some results on the use of FGMRES to stabilize such methods.

Randomized Inner-Product Free Krylov Solvers for Inverse Problems

Malena Sabaté Landman & Ariana N. Brown, Julianne Chung, James G. Nagy *(University of Oxford)*

Iterative Krylov projection methods have become widely used for solving large-scale linear inverse problems. However, methods based on orthogonality can cause the algorithms to break down in low precision due to information loss in the projections. Moreover, the computation of inner-products can also become costly when the number of iterations is high and is a bottleneck for parallelization. Recent works on inner-product free Krylov iterative algorithms alleviate these concerns, but they are quasi-minimal residual rather than minimal residual methods. This is a potential concern for inverse problems where the residual norm provides critical information from the observations via the likelihood function, and we do not have any way of controlling how close the quasi-norm is from the norm we want to minimize.

In this talk, I will introduce a new class of Krylov methods which combines (i) a generalization of the inherently inner-product free Hessenberg method for generating a solution subspace and (ii) a randomized sketch-and-solve approach for solving the resulting strongly overdetermined least-squares problem.

Numerical results show that the proposed algorithm can solve large-scale inverse problems efficiently and without requiring inner-products.

The numerical stability of sketched GMRES

Liam Burke & Erin Carson & Yuxin Ma *(Charles University)*

We will present results of a new backward stability analysis of sketched GMRES [Nakatsukasa and Tropp, SIAM J. Matrix Anal. Appl, 2024] for solving linear systems, and show that under certain assumptions, sketched GMRES is backward stable provided the condition number of the generated Krylov basis is not too large. Under additional assumptions, we then show that the stability of a restarted implementation of sketched GMRES can be independent of the condition number of the Krylov basis, and restarted sketched GMRES is backward stable. We also present sharper bounds that explain why the backward error produced by sketched GMRES can be small even in the cases where the Krylov basis is very ill-conditioned, which has been observed in the literature but not yet explained theoretically. We present results of numerical experiments to demonstrate the conclusions of our analysis, and also show that adaptively restarting where appropriate allows us to recover backward stability in sketched GMRES.

Low-rank approximation of parameter-dependent matrices via CUR decomposition

Taejun Park & Yuji Nakatsukasa *(University of Oxford)*

Low-rank approximation of parameter-dependent matrices $A(t)$ is an important task in the computational sciences, with applications in areas such as dynamical systems and the compression of series of images. In this talk, we introduce AdaCUR, an efficient randomized algorithm for computing low-rank approximations of parameter-dependent matrices using the CUR decomposition. The key idea of our approach is the ability to reuse column and row indices for nearby parameter values, improving efficiency. The resulting algorithm is rank-adaptive, provides error control, and has complexity that compares favourably with existing methods.

Adaptive randomized pivoting for low-rank approximation

Alice Cortinovis & Daniel Kressner *(University of Pisa)*

In this talk, we will present a new randomized algorithm for the column subset selection problem based on an adaptive leverage score sampling strategy. Our method, called Adaptive Randomized Pivoting (ARP), can be seen as a randomized counterpart to a recent deterministic approach proposed by Osinsky. It guarantees, in expectation, an approximation error that matches the optimal existence result in the Frobenius norm. Although the same guarantee can be achieved with volume sampling, ARP is less expensive.

We will highlight how this simple yet powerful strategy can be adapted to a range of tasks related to low-rank approximation, including the Discrete Empirical Interpolation Method, cross/skeleton approximation, and the Nyström approximation of positive semidefinite matrices. We'll also briefly describe a new deterministic variant for Nyström approximation that inherits strong error guarantees.

Small Sketches for Big Matrix Approximations

Nathaniel Pritchard & Taejun Park & Yuji Nakasukasa & Gunnar Martinsson *(University of Oxford)*

Low-rank approximations have become foundational to much of the improved scaling of techniques like clustering, machine learning, optimization, and uncertainty quantification. Classically, practitioners compute such low-rank approximations using the truncated SVD. However, owing to poor computational scaling, alternative approaches to forming low-rank approximations are of increasing interest. One such approach is the CUR decomposition, which forms a low-rank approximation using direct row and column subsets of the matrix. Because the CUR uses direct subsets of the matrix, it is often better able to preserve native matrix structures like sparsity or nonnegativity and in some data science contexts, even be more interpretable. Despite these benefits, most effective approaches to forming CUR approximations require a priori knowledge of the matrix's rank, an impractical requirement. This talk will present IterativeCUR, an accurate, scalable rank-adaptive approach that produces CUR approximations using only one small sketch of the matrix. It also will use rigorous experiments to show how IterativeCUR outperforms state-of-the-art CUR approaches without a loss in accuracy.

Near-optimal hierarchical matrix approximation from matrix-vector products

Diana Halikias & Tyler Chen, Feyza Duman-Keles, Cameron Musco, Chris Musco, David Persson *(Cornell University)*

Can one recover a matrix from only matrix-vector products? If so, how many are needed? We will consider the matrix recovery problem for the class of hierarchical rank-structured matrices. This problem arises in scientific machine learning, where one wishes to recover the solution operator of a PDE from only input-output pairs of forcing terms and solutions. Peeling algorithms are the canonical method for recovering a hierarchical matrix from matrix-vector products, however their recursive nature poses a potential stability issue which may deteriorate the overall quality of the approximation. Our work resolves the open question of the stability of peeling. We introduce a robust version of peeling and prove that it achieves low error with respect to the best possible hierarchical approximation to any matrix. This analysis relies on theory for low-rank approximation, as well as the surprising result that the Generalized Nyström method is more accurate than the randomized SVD algorithm in this setting.

Extracting Accurate Singular Values from Approximate Singular Subspaces

Lorenzo Lazzarino *(University of Oxford)* & Hussam Al Daas *(Scientific Computing, STFC-UKRI)* & Yuji Nakatsukasa *(University of Oxford)*

Given (orthonormal) approximations to the left and right subspaces spanned by the leading singular vectors of a matrix A, we discuss methods to approximate the leading singular values of A and study their accuracy. In particular, we focus our analysis on the generalized Nyström approximation, as surprisingly, it is able to obtain significantly better accuracy than classical methods, namely Rayleigh-Ritz and (one-sided) projected SVD. A key idea of the analysis is to view the methods as finding the exact singular values of a perturbation of A. In this context, we derive a matrix perturbation result that exploits the structure of such 2×2 block matrix perturbation. We then obtain bounds on the accuracy of the extracted singular values. This leads to sharp bounds that predict well the approximation error trends and explain the difference in the behavior of these methods. Our theoretical results translate into practical insights on how best to approximate singular values given approximate subspaces. Numerical experiments highlight how the derived bounds exhibit tighter estimates than classical bounds, effectively capturing the trends observed

empirically. For instance, the bounds reflect a more gradual change in error across the leading singular values.

References

[1] L. Lazzarino, H. Al Daas, and Y. Nakatsukasa, *Matrix perturbation analysis of methods for extracting singular values from approximate singular subspaces*, 2024, `https://arxiv.org/abs/2409.09187`.

Randomized algorithms for streaming low-rank approximation in tree tensor network format

Alberto Bucci *(Charles University)* & Gianfranco Verzella *(University of Geneva)*

Tensor decomposition is crucial because it provides compact representations of multi-dimensional data, reducing storage and computational costs while preserving essential features. It enables efficient data analysis, such as uncovering hidden patterns, correlations, or structures in complex datasets. This has broad applications in areas like machine learning, signal processing, and scientific computing.

In this talk, we present the tree tensor network Nyström (TTNN), an algorithm that extends recent research on streamable tensor approximation, such as for Tucker and tensor-train formats, to the more general tree tensor network format, enabling a unified treatment of various existing methods. Our method retains the key features of the generalized Nyström approximation for the low-rank approximation of matrices, that is randomized, single-pass, streamable, and cost-effective. We will also introduce a sequential variant of the algorithm, referred to as sequential tree tensor network Nyström (STTNN), which offers better performance for dense tensors. Furthermore, both algorithms are well-suited for the recompression or rounding of tensors in the tree tensor network format. The numerical experiments highlight the efficiency and effectiveness of the proposed methods.

References

[1] A. B., G. Verzella, (2024). Randomized Algorithms for Streaming Low-Rank Approximation in Tree Tensor Network Format, arXiv preprint.

Minisymposium M8

Recent developments in numerical integration, function approximation, and their applications in uncertainty quantification

Organisers
Yoshihito Kazashi and Yuya Suzuki

Comparing scale parameter estimators for Gaussian process regression: cross validation and maximum likelihood

Motonobu Kanagawa *(EURECOM)*

Gaussian process (GP) regression is a Bayesian nonparametric method for regression and interpolation, offering a principled way of quantifying the uncertainties of predicted function values. For the quantified uncertainties to be well-calibrated, however, the kernel of the GP prior has to be carefully selected. In this talk, we theoretically compare two methods for choosing the kernel in GP regression: cross-validation and maximum likelihood estimation. Focusing on the scale-parameter estimation of a Brownian motion kernel in the noiseless setting, we prove that cross-validation can yield asymptotically well-calibrated credible intervals for a broader class of ground-truth functions than maximum likelihood estimation, suggesting an advantage of the former over the latter.

Error estimation and superconvergence in kernel interpolation

Toni Karvonen *(Lappeenranta–Lahti University of Technology LUT)*

Computable error estimates for kernel interpolation can be derived from the equivalent Gaussian process (GP) framework by equipping the positive-definite kernel with a magnitude parameter and estimating this parameter with a statistical technique, such as maximum likelihood or cross-validation. Superconvergence refers to the phenomenon where a numerical method converges faster than expected if the problem it tries to solve is sufficiently nice. For example, one can view the quadratic convergence of the trapezoidal rule for twice differentiable functions as an instance of superconvergence. In this talk I review recent results on the superconvergence of kernel interpolation and discuss the implications these results have on error estimation via the GP framework. The talk is based on a number of joint papers with Tizian Wenzel, Gabriele Santin, Motonobu Kanagawa, Masha Naslidnyk, Maren Mahsereci, Filip Tronarp, George Wynne, Simo Särkkä

and Chris Oates.

Quasi-Monte Carlo for Bayesian shape inversion with Gevrey regular domain deformations

Max Orteu, Ana Djurdjevac, Vesa Kaarnioja, Claudia Schillings *(Freie Universität Berlin)*

We consider the application of a quasi-Monte Carlo cubature rule to Bayesian shape inversion subject to the Poisson equation under Gevrey regular parameterizations of domain uncertainty. We analyze the parametric regularity of the associated posterior distribution and design randomly shifted rank-1 lattice rules which can be shown to achieve dimension-independent, faster-than-Monte Carlo cubature convergence rates for high-dimensional integrals over the posterior distribution. In addition, we consider the effect of dimension truncation and finite element discretization errors for this model. Finally, a series of numerical experiments are presented to validate the theoretical results.

L_2-approximation using median lattice algorithms

Zexin Pan & Peter Kritzer, Takashi Goda *(RICAM)*

This talk presents a novel L_2-approximation algorithm for functions in weighted Korobov spaces, eliminating the need for prior knowledge of the smoothness parameter α and coordinate weights. By leveraging recent advances in median quasi-Monte Carlo methods, we construct approximations with nearly optimal convergence rates $O(n^{-\alpha})$, thereby surpassing the $O(n^{-\alpha/2})$ rates of classical lattice-based methods. Furthermore, a data-driven screening mechanism automatically identifies dominant Fourier coefficients and circumvents the curse of dimensionality in high-dimensional weighted spaces.

Optimal numerical integration over the real line: Möbius-transformed trapezoidal rule

Yuya Suzuki, Nuutti Hyvönen *(Aalto University)* & Toni Karvonen *(LUT)*

Recently, it has been proved that the well-known Gauss-Hermite quadrature is suboptimal. In this talk, we present a new numerical integration method, Möbius-transformed trapezoidal rule, for integration over the real line with a general class of weights. We prove that our method attains the optimal rate of convergence automatically if the integrand function lives in a weighted Sobolev space. Our algorithm only requires the ability to evaluate the weight at the selected nodes, and it does not require sampling from a probability measure defined by the weight nor information on its derivatives. In particular, we show that the Möbius transformation, as a change of variables between the real line and the unit circle, sends a function in the weighted Sobolev space to a periodic Sobolev space with the same smoothness. Since there are various results available for integrating and approximating periodic functions, we also describe several extensions of the Möbius-transformed trapezoidal rule, including function approximation via trigonometric interpolation, integration with randomized algorithms, etc. This talk is based on:

Y.S., N. Hyvönen, and T. Karvonen. "Möbius-transformed trapezoidal rule". Math. Comp. (2025). doi: 10.1090/mcom/4084

Convergence Rates of Randomized Quasi-Monte Carlo Methods under Various Regularity Conditions

Yang Liu *(King Abdullah University of Science and Technology)*

In this work, we analyze the convergence rate of randomized quasi-Monte Carlo (RQMC) methods under Owen's boundary growth condition (Owen, 2006) via spectral analysis. We examine the RQMC estimator variance for two commonly studied sequences—the lattice rule and the Sobol' sequence—using the Fourier transform and Walsh–Fourier transform, respectively. Under certain regularity conditions, our results reveal that the asymptotic convergence rate of the RQMC estimator's variance closely aligns with the exponent specified in Owen's boundary growth condition for both sequence types. We also provide an analysis for certain discontinuous integrands.

In addition, we investigate the L^p integrability of weak mixed first-order derivatives of the integrand and study the convergence rates of scrambled digital nets. We demonstrate that the generalized Vitali variation with parameter $\alpha \in \left[\frac{1}{2}, 1\right]$ from Dick and Pillichshammer (2010) is bounded above by the L^p norm of the weak mixed first-order derivative, where $p = \frac{2}{3-2\alpha}$. Consequently, when the weak mixed first-order derivative belongs to L^p for $1 \leq p \leq 2$, the variance of the scrambled digital nets estimator converges at a rate of $\mathcal{O}\left(N^{-4+\frac{2}{p}} \log^{s-1} N\right)$. Together, these results provide a comprehensive theoretical framework for understanding the convergence behavior of RQMC methods and scrambled digital nets under various regularity as-

sumptions.

References

[1] Liu, Y. (2024). Randomized quasi-Monte Carlo and Owen's boundary growth condition: A spectral analysis. To appear in IMA Journal of Numerical Analysis.

[2] Liu, Y. (2025). Integrability of weak mixed first-order derivatives and convergence rates of scrambled digital nets. Journal of Complexity, Volume 89, 2025, 101935.

Minisymposium M9

Recent Advances in Numerical Methods for Modern Materials

Organisers
Heiko Gimperlein and Ruma Rani Maity

Lowest-order nonstandard FEM for Extended Fisher Kolmogorov Equations

Neela Nataraj *(Indian Institute of Technology Bombay)*, Avijit Das, Gopikrishnan Remesan

The talk discusses lowest-order nonstandard finite element methods for space discretisation and backward Euler scheme for time discretisation of the extended Fisher–Kolmogorov equation with clamped boundary conditions. Spatial discretisation employs popular piecewise quadratic schemes based on triangles, namely, the Morley, the discontinuous Galerkin, and the C^0 interior penalty schemes. Based on a smoother defined for a piecewise smooth input function by a generalized Morley interpolation followed by a companion operator J, a Ritz projection is defined. A set of abstract hypotheses establish the approximation properties of the Ritz projection operator. The approach allows for an elegant semidiscrete and fully discrete error analysis with minimal regularity assumption on the exact solution. Error estimates for both the semidiscrete and fully discrete schemes are presented. The numerical results validate the theoretical estimates and demonstrate the capability of the discontinuous Galerkin method to approximate the solution, even for non-smooth initial condition.

Solution Landscapes in the Landau-de Gennes Theory for Nematic Liquid Crystals

Apala Majumdar *(University of Strathclyde)*

Liquid crystals are classical examples of partially ordered materials, that combine fluidity with the ordering characteristics of conventional solids to yield exceptionally responsive soft materials. Nematic liquid crystals are the simplest type of liquid crystals that exhibit long-range orientational ordering or have special material directions. Consequently, nematics are anisotropic materials with strong direction-dependent responses to external stimuli, making them popular working materials for an array of applications in science and technology. In this talk, we review the powerful continuum Landau-de Gennes theory for nematic liquid crystals. The admissible configurations are classical solutions of the associated Euler-Lagrange equations a system of five elliptic, nonlinear and coupled partial differential equations. We discuss numerical methods for canvassing the stable and unstable solutions of the Euler-Lagrange equations, and pathways between them to reveal the corresponding solution landscapes for benchmark examples. The solution landscapes hold crucial information about the static and dynamic properties of confined nematic systems, relevant for modern experiments and applications and we give some examples to this effect. This is joint work with Yucen Han, Baoming Shi and Lei Zhang.

Accelerated gradient flows in projection-free approximation of some nonconvex constrained variational problems

Shuo Yang *(Beijing Institute of Mathematical Sciences and Applications)* & Guozhi Dong, Zikang Gong, Hailong Guo, Ziqing Xie

In recent years, there has been many numerical explorations on non-convex constrained energy minimization problems, including models for nematic liquid crystals and large spontaneous deformation of materials. The projection-free gradient flow that deals with the constraint by conducting tangent space update has been widely adopted and analyzed. In our recent works, we improve such schemes by introducing momentum terms and combining it with high order BDF methods. Our new algorithms exhibit acceleration effect and a higher order constraint consistency.

A non conformal method for hyperelastic problem combined with neural network

V. Lleras *(IMAG, University of Montpellier)* & M. Duprez *(INRIA MIMESIS)* & A. Lozinski *(LMB, University of Franche-Comté)* & V. Vigon *(IRMA, University of Strasbourg)* & K. Vuillemot *(IMAG, University of Montpellier and INRIA MIMESIS)*

In this presentation we will detail a new machine learning approach combining a non conformal finite element method called ϕ-FEM [2] and the Fourier Neural Operator (FNO), a learning mapping operator [4]. The FNO based on discrete fast Fourier transform relies on an iterative architecture and takes a step size much bigger than is allowed in numerical methods. On the other side, ϕ-FEM, a finite element method with an immersed boundary approach using a level-set function, has an optimal convergence theoretically and numerically for multiple examples [1,2]. The key idea of our combined method [3] is to address the challenging scenario of varying domains, where each problem is solved on a different geometry. The considered domains are defined by level-set functions due to the use of the ϕ-FEM approach. These two methods are compatible since ϕ-FEM is a precise non-conforming finite element method, that can be used on cartesian grids, as required by the FNO that will be used. We will show numerical results for non linear equations like hyperelastic materials.

References:

[1] S. Cotin, M. Duprez, V. Lleras, A. Lozinski, and K. Vuillemot, *ϕ-FEM: an efficient simulation tool using simple meshes for problems in structure mechanics and heat transfer.* In Partition of Unity Methods (Wiley Series in Computational Mechanics) 1st Edition. Wiley, Nov. 2022.

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

[3] M. Duprez, V. Lleras, A. Lozinski, V. Vigon and K. Vuillemot, *ϕ-FEM-FNO: a new approach to train a Neural Operator as a fast PDE solver for variable geometries*, soumis.

[4] Z. Li, D. Z. Huang, B. Liu, and A. Anandkumar, *Fourier neural operator with learned deformations for PDEs on general geometries.* J. Mach. Learn. Res., 24(1), 2024.

A decoupled, convergent, and fully linear nodal projection free integrator for the Landau-Lifshitz-Gilbert equation including magnetostriction

Hywel Normington & Michele Ruggeri *(University of Strathclyde)*

The mechanical and magnetic properties of ferromagnetic materials are strongly coupled. Applying a stress to a ferromagnetic material changes the magnetic state, and applying a magnetic field deforms it. These fall collectively under the phenomena of "magnetostriction". We consider the coupled system of the Landau-Lifshitz-Gilbert (LLG) equation and conservation of momentum to describe magnetostrictive processes. For this nonlinear system of time-dependent partial differential equations, we present a decoupled and unconditionally convergent integrator based on linear finite elements in space and a one-step method in time. Compared to previous works on this problem, for our method, we prove a discrete energy law that mimics that of the continuous problem. Moreover, we do not employ a nodal projection to impose the unit-length constraint on the discrete magnetization, so that the stability of the method does not require weakly acute meshes. Furthermore, our integrator and its analysis hold for a more general setting, including body forces and traction, and a more general representation of the magnetostrain.

Numerical analysis for constrained and unconstrained Q-tensor energies for nematic liquid crystals

Ruma R. Maity (University of Innsbruck) & Heiko Gimperlein, Apala Majumdar, Neela Nataraj

Liquid crystals are anisotropic electro-optical materials with characteristics of both liquid and crystalline phases. Widely known for their use in display technology, recent advances have expanded their applications to include biological sensors, soft robotics, smart windows, and advanced optical devices. Mathematically, the classical Landau-de Gennes model encodes the properties of a liquid crystal in terms of the Q-tensor order parameter that satisfies a semilinear elliptic boundary value problem involving a nonlinear nonconvex potential function. In this talk, we discuss finite element approximation framework for the Landau-de Gennes Q-tensor energies for nematic liquid crystals, incorporating the anisotropy of the elastic energy and the Ball-Majumdar singular potential. This potential imposes essential physical constraints on the eigenvalues of the Q-tensor, ensuring realistic modeling. We discuss a priori error analysis to guarantee discrete local solutions near a regular root

of the nonlinear elliptic partial differential equations with non-homogeneous boundary conditions associated with Landau-de Gennes energies.
Numerical experiments support the optimal convergence estimates.

Minisymposium M10

Special Numerical Linear Algebra: Numerical advances at the interface of linear algebra and special functions

Organisers
Timon S Gutleb and Marcus Webb

Parameterizing Intersecting Surfaces via Invariants

Timon S. Gutleb *(University of Leeds)*, Rhyan Barrett, Julia Westermayr, Christoph Ortner

Conical intersections play a crucial role in determining the dynamics of molecules and materials upon light excitation, molecular orbitals and material band structure. In the relevant context of high-dimensional non-smooth hyper-surfaces, common machine learning models perform poorly. Here, we introduce and analyse numerical companion matrix methods for the reconstruction of hypersurfaces with crossings from smooth interpolants given unordered or, without loss of generality, value-sorted data.

Low Rank Approximation of Analytic Kernels

Marcus Webb *(University of Manchester)*

This talk is about the existence and computation of low rank approximations to matrices coming from samples of a kernel $K(x, y)$ that can be analytically continued in one of its variables to a large region of the complex plane. From one abstract theorem we are able to generalise and in some cases improve upon several recent results about the decay of singular values and low rank approximation in various norms. The results are applied to develop algorithms for fast orthogonal polynomial transforms and fast discrete Hankel transforms.

Parallelising PDEs using Representation Theory

Sheehan Olver *(Imperial College London)*

If a partial differential operator is invariant under a symmetry group (permutations, rotations, reflections, etc.) then it can be coupled by discretising with a so-called *symmetry-adapted basis*, built from irreducible representations, the basic building blocks of representation theory. In this talk we explore this phenomena using symmetry-adapted multivariate orthogonal polynomials to discretise Schrödinger equations with potentials invariant under permutations or the octohedral symmetry group for the cube.

Matrix equations and orthogonal polynomials

Richard Mikael Slevinsky & Karim Gumerov & Gabriel Hamm & Samantha Rigg *(University of Manitoba)*

It is well known that matrices with low Hessenberg-structured displacement rank enjoy fast algorithms for certain matrix factorizations. We show how $n \times n$ principal finite sections of the Gram matrix for the orthogonal polynomial measure modification problem has such a displacement structure, unlocking a collection of fast algorithms for computing connection coefficients (as the upper-triangular Cholesky factor) between a known orthogonal polynomial family and the modified family. In general, the $\mathcal{O}(n^3)$ complexity is reduced to $\mathcal{O}(n^2)$, and if the symmetric Gram matrix has upper and lower bandwidth b, then the $\mathcal{O}(b^2 n)$ complexity for a banded Cholesky factorization is reduced to $\mathcal{O}(bn)$. Next, we will extend this basic result to a matrix equation for the Sobolev–Gram matrix which has a number of terms proportional to the order of the corresponding Sobolev inner product. Finally, we will discuss the structure of Gram matrices of multivariate orthogonal polynomials. These multivariate Gram matrices are endowed with a block structure, and they satisfy a number of simultaneous matrix equations equal to the dimension of the domain.

Orthogonal polynomials and combinatorics

Geoff Vasil *(University of Edinburgh)*

One of the best things about classical orthogonal polynomials (OP) is their remarkable properties involving continuous operations like differentiation and multiplication. Originally intended to solve continuous problems of analysis (e.g. differential equations) and physical applications (e.g. tides, electromagnetism and quantum mechanics), classical and non-classical polynomials have also found great traction in modern probability (e.g. Markov chains). However, upon closer inspection, the innards of many OP families contain abundant factorials, binomial coefficients and other famous combinatorial trappings. Compared to their analytical properties, what OP families say about counting remains much less explored. This talk will

inject a little bijective interpretation into the OP discourse. In the long term, a much deeper understanding will hopefully produce a virtuous feedback that influences all areas where OP casts shadows.

A sparse spectral method on domains bounded by algebraic curves

Jiajie Yao *(University of Leicester)* & Marco Fasondini *(University of Leicester)* & Sheehan Olver *(Imperial College London)*

We develop a sparse spectral method for solving partial differential equations on a broad class of two-dimensional geometries bounded by algebraic curves, referred to as generalised Koornwinder domains. The numerical method utilises a bivariate Koornwinder polynomial basis, built from new families of univariate semiclassical orthogonal polynomials whose operator matrices are computed hierarchically with optimal complexity. In the discretisation of PDEs, this basis allows for sparse representations of conversion (change-of-basis), multiplication and differentiation operators, while also enabling fast analysis and synthesis transforms. We further propose a quadrature-free Stieltjes-type algorithm to generate a set of bivariate orthogonal polynomials on generalised Koornwinder domains, with potential applications in constructing a sparse spectral element method.

A sparse *hp*-finite element method for piecewise-smooth differential equations with periodic boundary conditions

Daniel VandenHeuvel & Sheehan Olver *(Imperial College London)*

In this talk, I discuss an efficient *hp*-finite element method developed for piecewise-smooth differential equations with periodic boundary conditions, using orthogonal polynomials defined on circular arcs. The operators derived from this basis are banded and achieve optimal complexity regardless of h or p, both for building the discretisation and solving the resulting linear system in the case where the operator is symmetric positive definite. The basis serves as a useful alternative to other bases such as the Fourier or integrated Legendre bases, especially for problems with discontinuities.

The Akhiezer iteration for matrix functions and Sylvester equations

Cade Ballew & Thomas Trogdon & Heather Wilber *(University of Washington)*

We present an iterative method for solving indefinite linear systems and computing matrix functions via orthogonal polynomial expansions. We utilize orthogonal polynomials for weight functions supported on intervals that roughly correspond to the eigenvalues of the matrix in question. When two or more intervals are considered, extensions of the Chebyshev polynomials, often called the Akhiezer polynomials, are employed. The iterative method achieves a provable geometric rate of convergence and applies in settings where classical polynomial approximations behave poorly and are therefore not applicable. Applied to the matrix sign function, the method yields a fast inverse-free iteration for solving Sylvester matrix equations.

Sampling theory for function approximation with numerical redundancy

Astrid Herremans & Daan Huybrechs *(KU Leuven)*

In function approximation, it is standard to assume the availability of an orthonormal basis for computations to ensure that numerical errors are negligible. However, this assumption is often violated in practice. In this work, we discard it and study how numerical phenomena influence computations with non-orthogonal bases. To characterize when rounding errors become significant, we introduce the concept of numerical redundancy: a set of functions is numerically redundant if it spans a lower-dimensional space when analysed numerically rather than analytically. Previous research has shown that numerical redundancy leads to a gap between the accuracy of computed approximations and the best approximation. Here, we present a complementary positive result: numerical redundancy can also significantly reduce the amount of data required for accurate approximation. More specifically, we show that the required amount of data only depends on the numerical dimension of the basis.

Minisymposium M11

Numerical analysis for nonlinear PDEs
Organisers
Soeren Bartels and Max Jensen

Asymptotic compatibility of parametrized optimal design problems

Abner J. Salgado & Tadele Mengesha & Joshua M. Siktar *(University of Tennessee)*

We study optimal design problems where the design

corresponds to a coefficient in the principal part of the state equation. The state equation, in addition, is parameter dependent, and we allow it to change type in the limit of this (modeling) parameter. We develop a framework that guarantees asymptotic compatibility, that is unconditional convergence with respect to modeling and discretization parameters to the solution of the corresponding limiting problems. This framework is then applied to two distinct classes of problems where the modeling parameter represents the degree of nonlocality. Specifically, we show unconditional convergence of optimal design problems when the state equation is either a scalar-valued fractional equation, or a strongly coupled system of nonlocal equations derived from the bond-based model of peridynamics.

Weak and strong convergence of a BDF2-type integrator for the Landau–Lifshitz–Gilbert equation in micromagnetics

Michele Aldé, Michael Feischl & Dirk Praetorius *(TU Wien)*

We consider the Landau–Lifshitz–Gilbert (LLG) equation, a nonlinear partial differential equation that models time-dependent micromagnetic phenomena. We propose a full discretization scheme based on first-order finite elements in space and an implicit BDF2-type two-step method in time. Despite the nonlinearities of LLG, only one linear system must be solved per time-step. This scheme is, to our knowledge, the first BDF2-type integrator for LLG that guarantees both unconditional weak convergence to weak solutions of LLG, as well as optimal strong convergence in the presence of smooth solutions. Specifically, we prove a-priori error estimates of order $\mathcal{O}(h+k^2)$, where k and h denote the time-step size and spatial mesh-size, respectively — that is, second-order in time and first-order in space. Numerical experiments illustrate and confirm the theoretical results.

A Nitsche method for fluid flow with nonlinear and dynamic boundary conditions

Tabea Tscherpel & Alexei Gazca & Franz Gmeineder & Erika Maringová Kokavcová *(Technical University of Darmstadt)*

Non-Newtonian fluids often exhibit boundary conditions that are significantly more complex than standard no-slip or Navier-slip conditions. Much like the relationship between shear rate and stress tensor, the boundary behaviour can be interpreted as a constitutive relation. As such, one may encounter boundary conditions that are nonlinear, non-coercive, non-monotone or dynamic.

In this talk, we present a mixed finite element method to approximate incompressible fluid flow under such boundary conditions. To impose the boundary conditions we employ a Nitsche penalisation method. This approach is particularly advantageous, since direct enforcing of the boundary conditions on curved domains may lead to a Babuška-type paradox.

For extensions to implicit boundary conditions, such as the Tresca or stick-slip boundary conditions we refer to a talk by A. Gazca.

Guaranteed upper bounds for iteration errors and modified Kačanov schemes via discrete duality

Johannes Storn & Lars Diening *(Leipzig University)*

We apply duality theory to discretized convex minimization problems to obtain computable guaranteed upper bounds for the distance of given discrete functions and the exact discrete minimizer. Furthermore, we show that the discrete duality framework extends convergence results for the Kačanov scheme to a broader class of problems.

Weighted Aleksandrov Estimates

Lukas Gehring *(Friedrich-Schiller-Universität Jena)*

We present a stronger version of the classical Aleksandrov estimate for the Monge–Ampère operator. Instead of the Monge–Ampère measure of the whole domain, a weight function is integrated with respect to the Monge–Ampère measure and this weight function decays to the boundary – roughly speaking with a certain power of the distance to the boundary. The inequality implies a stronger Aleksandrov–Bakelman–Pucci principle for uniformly elliptic equations and an extension of the theorem about existence of solutions of the Dirichlet problem of the Monge–Ampère equation. Additionally, there is a generalization for the k-Hessian measure. The results expand those in "Weighted Aleksandrov estimates: PDE and stochastic versions" by N.V. Krylov.

From Monge-Ampère to Stochastic Optimal Control

Ivan Majić & Max Jensen *(UCL)*

A Monge-Ampère equation is a nonlinear second-order partial differential equation involving the determinant of the Hessian matrix of the unknown function. It

arises in many fields, such as Optimal Transport. Under appropriate conditions, the Monge-Ampère equation has an equivalent Hamilton-Jacobi-Bellman (HJB) equation formulation in the classical and viscosity solution sense. In this talk, we will look at a model Monge-Ampère equation and its corresponding HJB equation and identify the Stochastic Optimal Control (SOC) problem which is well-posed and has the same solution as the HJB equation. We will discuss the proof of the existence of weak controls for this SOC problem and showcase attempts at solving it numerically using Reinforcement Learning. Finally, we will look at some more complicated examples of the Monge-Ampère equation with lower order terms and discuss why the same method does not apply and we will consider utilising Markov Decision Processes instead.

Minisymposium M12

Recent advances in numerical linear algebra with insights from scientific machine learning

Organisers

James Jackaman and Jemima Tabeart

Dimensionality Reduction Techniques for Global Bayesian Optimisation

Paz Fink Shustin & Luo Long & Coralia Cartis *(University of Oxford)*

Bayesian Optimisation (BO) is a state-of-the-art global optimisation technique for black-box problems where derivative information is unavailable and sample efficiency is crucial. However, improving the general scalability of BO has proved challenging. Here, we explore Latent Space Bayesian Optimisation (LSBO), that applies dimensionality reduction to perform BO in a reduced-dimensional subspace. While early LSBO methods used (linear) random projections (Wang et al., 2013), we employ Variational Autoencoders (VAEs) to manage more complex data structures and general DR tasks. Building on Grosnit *et al.* (2021), we analyse the VAE-based LSBO framework, focusing on VAE retraining and deep metric loss. We suggest a few key corrections in their implementation, originally designed for tasks such as molecule generation, and reformulate the algorithm for broader optimisation purposes. Our numerical results show that structured latent manifolds improve BO performance. Additionally, we examine the use of the Matérn-$\frac{5}{2}$ kernel for Gaussian Processes in this LSBO context. We also integrate Sequential Domain Reduction (SDR), a standard global optimization efficiency strategy, into BO. SDR is included in a GPU-based environment using *BoTorch*, both in the original and VAE-generated latent spaces, marking the first application of SDR within LSBO.

Learning efficient solvers for time dependent PDEs on the sphere

Eike Müller *(University of Bath)* & Katherine MacKenzie *(University of Strathclyde)*

Recently, machine learning approaches to numerical weather prediction (NWP) such as PanguWeather [Bi et al., 2023] and GraphCast [Lam et al., 2023] have attracted significant attention since they can produce forecasts much faster than traditional codes. GraphCast and other models [Keisler, 2022] use an encoder-processer-decoder architecture: a learnable embedding maps the unknowns of the discretised PDEs to a latent space. The resulting low-dimensional state is then evolved via message passing on a Graph Neural Network, before being mapped back to a function on the sphere which represents the solution at the final time. In this talk I will discuss a variant of this approach in which the processor on the latent space is replaced by the solution of an ODE with a learnable forcing function in the spirit of the Neural ODE approach by [Chen et al., 2018]. This more physical design has the potential to improve stability and interpretability. I will discuss an implementation which uses the recently developed interface between the Firedrake finite element library and the PyTorch machine learning framework [Bouziani and Ham, 2023].

Iterative Block Matrix Inversion Algorithm with Applications to Covariance Matrices

Ann Paterson & Jennifer Pestana & Victorita Dolean *(University of Strathclyde)*

Obtaining the inverse, or selected elements of the inverse of a large symmetric positive definite matrix $\mathcal{A} \in \mathbb{R}^{n\times n}$ arises in a number of fields, including computational physics, machine learning and Bayesian statistics. In particular, a number of important computations in statistics require the inverse of positive definite matrices, or certain sub-matrices of these, e.g., within Gaussian process regression. Here we present a novel algorithm which is designed to approximate the inverse of a large symmetric positive definite matrix. An iterative process of partitioning the matrix $\mathcal{A}$ and using block matrix inversion is repeated, until the approximated inverse $\mathcal{H} = \mathcal{A}^{-1}$ reaches a satisfactory level of accuracy. We demonstrate that the two-block, non-overlapping approach converges for any positive definite matrix, while numerical results provide strong evidence that the multi-block, overlapping approach

also converges for such matrices.

Learning components of multilevel preconditioners

Scott MacLachlan *(Memorial University of Newfoundland)*

Multilevel preconditioners are well-known to provide optimal algorithms for the solution of many discretized PDEs. They are also well-known to be sensitive to many algorithmic choices, such as relaxation parameters in a multigrid method or transmission conditions in a domain-decomposition approach. In this talk, I will discuss the development and analysis of machine learning tools to help make these choices. One key question in this development is how to measure performance of preconditioned iterations in a loss function, and several options will be presented. Numerical examples will demonstrate the effectiveness of the overall approach.

Efficient gradient-based methods for bilevel learning via recycling Krylov subspaces

Sebastian J. Scott & Matthias J. Ehrhardt & Silvia Gazzola *(University of Würzburg)*

A data-driven way to determine hyperparameter values, such as those of a parametrised regulariser, is via a nested optimisation framework known as bilevel learning. Employing a gradient-based method to solve the bilevel learning problem is computationally challenging, as each gradient requires both a solution of a minimisation problem and a linear system solve. Since these systems do not change much between iterations, it can be a computational gain to employ recycling Krylov subspace methods, wherein information from one linear system solve is re-used to solve the next linear system. While existing recycling strategies use eigenvector approximations called Ritz vectors, in this talk we propose a novel recycling strategy based on a new concept, Ritz generalised singular vectors, which acknowledge the bilevel setting and allows for a new stopping criterion that directly approximates the error of the associated gradient.

Computing the Posterior Mean in a Multi-output Gaussian Process for separable covariance

Sebastian Esche & Martin Stoll *(TU Chemnitz)*

Gaussian processes (GP) are a versatile tool in machine learning and computational science. We consider the case of multi-output Gaussian processes (MOGP) and present a low-rank approach for efficiently computing the posterior mean of a MOGP. Starting from low-rank spatio-temporal data we consider a structured covariance function, assuming separability across space and time. This separability, in turn, gives a decomposition of the covariance matrix into a Kronecker product of individual covariance matrices. Incorporating the typical noise term to the model then requires the solution of a large-scale Stein equation for computing the posterior mean. For this, we propose an efficient low-rank CG method adapted to the Kronecker product for solving the Stein equation. As a preconditioner, we employ the Sylvester equation solver KPIK, which we modify to handle Stein equations.

Minisymposium M13

Advanced numerical techniques for kinetic equations

Organisers

Giacomo Borghi and Andrea Medaglia

A BGK Model for Particle Swarm Optimization with Jumps

Hyesung Im & Giacomo Borghi & Lorenzo Pareschi *(Maxwell Institute for Mathematical Sciences and Department of Mathematics, School of Mathematical and Computer Sciences (MACS), Heriot-Watt University)*

Metaheuristic algorithms are powerful tools for global optimization, particularly for non-convex and non-differentiable problems where exact methods are often impractical. Among them, Particle Swarm Optimization (PSO) is a popular population-based method in which particles explore the search space by adjusting their velocities based on individual and collective experience. In this work, we study a PSO variant where velocities are updated via random jumps—a strategy used in several existing methods to enhance stochastic exploration. We formalize this approach by modelling the dynamics through a kinetic model of BGK type, offering a unified framework that accommodates general noise distributions, including heavy-tailed ones like Cauchy. Under suitable parameter scaling, the model reduces to the Consensus-Based Optimization (CBO) dynamics. For Gaussian noise in bounded domains, we prove propagation of chaos and convergence towards minimizers. Numerical results on benchmark problems validate the approach and highlight its connection to CBO.

A Parallel in time numerical method for the collisional Vlasov equation in the hyperbolic scaling

Tino Laidin & Thomas Rey *(Laboratoire de Mathématique Bretagne Atlantique)* & *(Université Côte (d'Azur)*

In this talk, I will present joint work with T. Rey on the development of a multiscale parareal method tailored for kinetic equations. Our objective is to significantly reduce the computational cost of fully kinetic simulations by employing a parallel-in-time framework. The parareal method, an iterative predictor-corrector scheme, leverages both coarse and fine time integrators. By exploiting the multiscale nature of kinetic models, we use a computationally inexpensive fluid solver as the coarse predictor and a more accurate, yet costly, kinetic solver as the fine corrector, applied to a collisional Vlasov equation.

Structure-preserving neural network surrogates for kinetic equations with uncertainty

Lorenzo Pareschi *(Heriot Watt University)*

Uncertainty quantification for kinetic equations with stochastic parameters presents major computational challenges due to the high dimensionality and nonlinearity of the models. Traditional Monte Carlo methods suffer from slow convergence and high variance, particularly when dealing with complex nonlinear models such as the Boltzmann equation. In this talk, we present a novel approach that integrates structure-preserving neural networks within a multifidelity asymptotic preserving framework to efficiently address these issues.

We introduce deep neural networks, trained in a physics-informed fashion, as low-fidelity surrogate models to reduce variance while preserving key physical properties of the solution, such as nonnegativity and entropy dissipation. In particular, we focus on a structure-preserving PINN, which enhances standard PINN approaches by embedding conservation properties directly into the learning process. The resulting hybrid algorithm, combining data-driven surrogates and high-fidelity solvers, allows for significant computational savings while maintaining accuracy in the estimation of statistical observables.

Numerical experiments, including homogeneous and non-homogeneous problems with uncertain initial conditions, demonstrate the effectiveness of our methodology. We show that the use of multiple control variates and structure-preserving neural networks can substantially outperform classical MC methods in terms of error reduction and computational cost.

This is a joint research with Wei Chen *(Xiamen University, Xiamen, China)*, Giulia Bertaglia and Giacomo Dimarco *(University of Ferrara, Ferrara, Italy)*

From Variance Reduction to Density Estimation: Interplay of Entropy and Moments

Mohsen Sadr *(ETH, Paul Scherrer Institute, Switzerland)*

In this talk, I review the concept of the maximum entropy principle for parametric density estimation and its relation to moments with two applications relevant to particle methods in kinetic theory: variance reduction and particle generation. First, I discuss the challenges with most variance reduction methods for particle codes in kinetic theory, including numerical instabilities in the collisional limit or bias in the rarefied regime. Among these, the importance sampling method that takes advantage of the correlation between non-equilibrium and the control variate processes using weights has gained attention in the literature, as it requires a minimal change in the base simulation code. However, the exact weight process becomes multiplicative for many kinetic models, including the Boltzmann and Fokker-Planck equations, leading to divergent weight spread as the particle distribution approaches equilibrium. In order to stabilize such a weight process, smoothers such as Kernel Density Estimation (KDE) are often deployed to resample weights subject to bias, as the moment conservation is ignored. In order to minimize the bias, I introduce a correction for the smoothed-out weight distribution by maximizing cross-entropy while enforcing the moment conservation using the method of Lagrange multipliers. This leads to a convex optimization problem which can be solved efficiently in a few iterations.

In the second part of the talk, I review the *moment problem* relevant to hybrid continuum/kinetic models, e.g. generating particles when only moments are known at the interface of particle and moment-based methods. Here, I address the ill-posedness of this problem and issues such as limits-of-realizability and ill-conditionality of the least biased parametric density estimator, i.e. maximum entropy distribution. In order to ensure existence, I show that the maximum entropy distribution can be regularized by redefining the underlying optimization problem using the Monge-Kantorovich formulation devised for the optimal transport problem, where the Wasserstein distance from the equilibrium distribution ensures existence of the posterior distribution. Using the variational calculus, we can find the form of the joint distribution function, where its target marginal satisfies

the Boltzmann equation up to the first order. This allows us to devise and solve a moment-based stochastic differential equation to generate samples that match the desired moments up to the statistical noise. Here, I show the accuracy and cost of the proposed sampling method in a wide range of rarefactions for the Boltzmann equation.

Hierarchical domain decomposition method for the multi-scale Boltzmann equation with geometry

Domenico Caparello & Lorenzo Pareschi & Thomas Rey *(Université Côte-d'Azur & University of Ferrara)*

In this work, we present a hierarchical domain decomposition method for the multi-scale Boltzmann equation based on moment realizability matrices, a concept introduced by Levermore, Morokoff, and Nadiga. This criterion is used to dynamically partition the two-dimensional spatial domain into three regimes: the Euler regime, an intermediate kinetic regime governed by the ES-BGK model, and the full Boltzmann regime. The key advantage of this approach lies in the use of Euler equations in regions where the flow is near hydrodynamic equilibrium, the ES-BGK model in moderately non-equilibrium regions where a fluid description is insufficient but full kinetic resolution is not yet necessary, and the full Boltzmann solver where strong non-equilibrium effects dominate, such as near shocks and boundary layers. This allows for both high accuracy and significant computational savings, as the Euler solver and the ES-BGK models are considerably cheaper than the full kinetic Boltzmann model. To ensure accurate and efficient coupling between regimes, we employ asymptotic-preserving (AP) numerical schemes and fast spectral solvers for evaluating the Boltzmann collision operator. Among the main novelties of this work are the use of a full 2D spatial and 3D velocity decomposition, the integration of three distinct physical regimes within a unified solver framework, and a parallelized implementation exploiting CPU multithreading. This combination enables robust and scalable simulation of multiscale kinetic flows with complex geometries.

Particle methods for kinetic equations with random inputs

Andrea Medaglia *(University of Oxford)*

The study of kinetic equations, such as those modelling plasmas, semiconductor devices, and multiagent systems, is crucial for understanding complex systems in diverse fields. At the kinetic scale, particle-based methods are widely used to capture the evolution of distribution functions in these systems exhibiting multiscale phenomena. However, in real-world applications, uncertainties in parameters like initial data and boundary conditions can significantly affect the behaviour of the solution.

To address these uncertainties, it is essential to incorporate random inputs into the model. This adds complexity, as it increases the dimensionality of the problem, known as the curse of dimensionality, and requires careful numerical treatment to maintain the physical properties of the solution, such as conservation laws, entropy dissipation, and large time asymptotic behaviour.

Recently, particle methods combined with stochastic Galerkin expansions have been developed to handle the random input space while preserving the key structural properties of kinetic equations. These methods offer spectral accuracy with respect to random parameters and are well-suited for capturing multiscale phenomena in high-dimensional settings. In this talk, we introduce this kind of particle-based methods and we present several numerical results with application to plasma physics, and semiconductor equations.

This is a joint work with Dr. R. Bailo, Prof. J.A. Carrillo, Prof. L. Pareschi, and Prof. M. Zanella.

Minisymposium M14

Numerical methods for PDEs on curved domains or surfaces

Organiser
Jiashun Hu

φ-FEM: an optimally convergent and easily implementable immersed boundary method for particulate flow and Stokes equations

Michel Duprez *(Inria)* & Vanessa Lleras *(University of Montpellier)* & Alexei Lozinski *(University Franche-Comté)* & Killian Vuillemot *(University of Montpellier)*

In this talk, we will present an immersed boundary method to simulate the creeping motion of a rigid particle in a fluid described by the Stokes equations discretized thanks to a finite element strategy on unfitted meshes, called φ-FEM, that uses the description of the solid with a level-set function. One of the advantages of our method is the use of standard finite element spaces and classical integration tools, while maintaining the optimal convergence (theoretically in the H^1 norm for the velocity and L^2 for pressure; numerically

also in the L^2 norm for the velocity). We will finish with some numerical illustrations.

Numerical analysis of BDF time stepping schemes with implicit extensions for the Stokes equations on evolving domains

Stefan Frei *(University of Konstanz)* & Erik Burman *(University College London)* & Andre Massing *(NTNU Trondheim)*

We consider time discretisation of the Stokes equations on a time-dependent domain $\Omega(t)$ in an Eulerian coordinate framework. Our work can be seen as an extension of the work by Lehrenfeld & Olshanskii [ESAIM: M2AN, 53(2):585-614, 2019], where BDF-type time-stepping schemes are analysed for a parabolic equation on time-dependent domains. For space discretisation, a geometrically unfitted finite element discretisation is applied in combination with Nitsche's method to impose boundary conditions. Physically undefined values of the velocities that will be needed in following time steps are extended implicitly by means of so-called *ghost penalty* stabilisations. We give some insights into the stability and the *a priori* error analysis in space and time, which is complicated by the fact that the velocity $u(t_{n-1})$ from the previous time t_{n-1} is not discrete divergence free with respect to the domain $\Omega(t_n)$ at the current time t_n. As a result, we obtain optimal error bounds for the velocities and a suboptimal error bound for pressure. Finally, the theoretical results are substantiated with numerical examples in three space dimensions.

A stabilized arbitrary Lagrangian–Eulerian sliding interface method for fluid-structure interaction with a rotating rigid structure

Yali Gao (Northwestern Polytechnical University) & **Jiashun Hu** *(Hong Kong Polytechnic University)* & Buyang Li *(Hong Kong Polytechnic University)*

We introduce a novel sliding interface formulation for fluid-structure interaction (FSI) between a rotating rigid structure and incompressible fluid, improving existing methodologies with a skew-symmetric Nitsche's stabilization term applied on an artificial sliding interface, alongside a rotational arbitrary Lagrangian-Eulerian framework. This innovative approach not only preserves the energy-dissipating property at the continuous level but also provides a robust foundation for further advancements in FSI modeling. Our methodology includes a first-order full discretization that maintains these critical energy-dissipating properties at the discrete level, ensuring numerical stability and accuracy. While prior contributions such as the original sliding interface method introduced by Bazilevs & Hughes (Comput. Mech., 43(1):143–150, 2008) have been significant, theoretical analyses such as the inf-sup condition on non-matching meshes have gone largely unaddressed. We fill this gap by proving the inf-sup condition within the context of the isoparametric finite element method (FEM), where meshes are not only non-matching but also overlapping, thus extending the applicability and robustness of our approach. Leveraging this inf-sup condition along with the inherent energy-dissipating properties, we establish the unique solvability of the fully discrete scheme. Through extensive numerical experiments, we illustrate the convergence, efficiency, and energy-dissipating property of the proposed method.

A new framework of high-order unfitted finite element methods using ALE maps for moving-domain problems

Chuwen Ma *(Shanghai Jiao Tong University)*

We present a generic framework for arbitrary Lagrangian–Eulerian unfitted finite element (ALE-UFE) methods for partial differential equations (PDEs) on time-varying domains. The ALE-UFE method shows great potential for developing high-order unfitted finite element methods. Its effectiveness is demonstrated through various moving-domain problems, including a linear problem with explicitly prescribed boundary (or interface) velocity, a PDE–domain coupled problem, and a problem involving topological changes in the domain. Numerical experiments show that both third- and fourth-order methods achieve optimal convergence on domains with smooth boundaries, but performance deteriorates when the domain undergoes topological changes.

ESFEM for the Lagrangian approach of the full Navier-Stokes equations on evolving surfaces

Achilleas Mavrakis & Charles M. Elliott *(University of Warwick)*

In this talk, we consider a fully discrete numerical method for the Lagrangian approach of the full Navier-Stokes posed on a smooth evolving closed surface in $\mathbb{R}^3$ with prescribed normal velocity. This method is based on the full evolving surface Navier-Stokes equations where the normal component of the velocity is enforced via an extra Lagrange multiplier λ. For the discrete formulation we employ a generalized Taylor-Hood evolving surface finite element pair $\mathcal{P}^{k_u} - \mathcal{P}^{k_{pr}} - \mathcal{P}^{k_\lambda}$ (ESFEM). Considering $k_\lambda = k_u$ we present a complete stability and error analysis, where optimal convergence is established for the velocity in an energy norm, with low regularity assumptions. With the same assumptions, we also show $L^2(L^2)$ stability

and optimal convergence for the two pressures. Assuming further regularity for the continuous velocity, we see that it is also possible to show optimal convergence estimates in the case where $k_\lambda = k_u - 1$, only for super-parametric evolving surface Taylor-Hood finite elements, that is, when for the geometric approximation $k_g = k_u + 1$ holds. Finally, we demonstrate numerical results that agree with our theoretical findings.

Random Walk Algorithm for Solving a Moving Boundary Problem Describing Diffusant Penetration into Rubber

Surendra Nepal, Magnus Ögren, Yosief Wondmagegne, Adrian Muntean *(Linnaeus University)*

For certain materials science scenarios arising in rubber technology, one-dimensional moving boundary problems with kinetic boundary conditions can reveal the large-time behavior of the diffusant penetration front, providing a direct estimate of the material's service life. Motivated by our interest in estimating how a finite number of diffusant molecules penetrate dense rubber, we propose a random-walk algorithm to numerically approximate both the concentration profile and the location of the sharp penetration front. The proposed scheme decouples the evolution system into two steps: (i) solving the ordinary differential equation that determines the speed of the moving boundary via an explicit Euler method, and (ii) solving the associated diffusion problem using a random walk method. To verify the accuracy of our random-walk algorithm, we compare the resulting approximations with computational results obtained from a suitable finite element approach with a controlled convergence rate. Our numerical results recover well penetration depth measurements of a controlled experiment designed specifically for this setting.

Optimal Convergence of an Arbitrary Lagrangian–Eulerian Finite Element Method for Fluid–Structure Interactions

Qiqi Rao & Buyang Li *(The Hong Kong Polytechnic University)* & Pengtao Sun *(University of Nevada Las Vegas)*

The optimal convergence analysis in $L^\infty(0,T;H^1)$ norm is achieved for a monolithic, arbitrary Lagrangian–Eulerian (ALE)-based mixed finite element method in fully discrete scheme, while solving the realistic fluid–structure interaction (FSI) problems with solution–driven moving interfaces. In addition to the finite element approximation errors, the geometric approximation errors due to the domain/interface motion and mesh evolvement are considered as well within the ALE frame. Moreover, an initial correction term is added to the employed backward Euler scheme in order to obtain the optimal error estimate in $L^\infty(0,T;H^1)$ norm. Numerical experiments in both two and three dimensions are carried out to validate the attained theoretical results.

Evolving surface finite elements for the Cahn-Hilliard equation with a logarithmic potential

Thomas Sales & Charles M. Elliott *(University of Warwick)*

Recently there has been much interest on partial differential equations on evolving domains, as motivated by applications in biology (for example in studying dynamics of lipid biomembranes) and physics (nanoporosity in electrolytic dealloying of binary alloys). In this talk we discuss recent results concerning the finite element approximation of an evolving surface version of the Cahn-Hilliard equation with a (singular) logarithmic potential. The theoretical results hinge on a geometric assumption on the evolving surface which we motivate before outlining the proof of error bounds, highlighting the key differences between results for a regular (polynomial) potential.

A Trace Finite Element Method for Navier–Stokes equations on evolving surfaces

Paul Schwering & Arnold Reusken *(RWTH Aachen University)*

In recent years there has been a strongly growing interest in PDEs posed on surfaces, in particular concerning physical principles related to these equations and tailor-made numerical discretization methods. One reason for this growing interest lies in the fact that these equations are used in the modeling of biological interfaces. In this talk we present a new finite element based method for the numerical approximation of the Navier-Stokes equations posed on evolving closed surfaces embedded in $\mathbb{R}^3$. The PDE system is as follows: For a known force term $\mathbf{f}$, a given initial surface $\Gamma(0)$ and an initial velocity $\mathbf{u}^0$ on $\Gamma(0)$, find the velocity field $\mathbf{u}$, the pressure p and the corresponding surface $\Gamma(t)$ satisfying

$$\begin{cases} \dot{\mathbf{u}} - \operatorname{div}_\Gamma \mathbf{E}_\Gamma(\mathbf{u}) + \nabla_\Gamma p - p\kappa\mathbf{n} = \mathbf{f} & \text{on } \Gamma(t), \\ \operatorname{div}_\Gamma \mathbf{u} = 0 & \text{on } \Gamma(t). \end{cases}$$

Here, $\mathbf{n}$ and κ are the normal vector and the mean curvature of the surface, $\dot{\mathbf{u}}$ denotes the material derivative of the velocity field, ∇_Γ and $\operatorname{div}_\Gamma$ represent the sur-

face gradient and divergence operator, and $\mathbf{E}_\Gamma(\mathbf{u})$ is the surface rate-of-strain tensor.

For these equations, one major challenge is the interplay of the velocity field defined by the PDE on $\Gamma(t)$ and the surface geometry evolution which depends on the velocity field. The evolution of the surface $\Gamma(t)$ itself is an unknown of the system. We represent the surface as the zero level of a level set function ϕ that fulfills the level set equation

$$\frac{\partial}{\partial t}\phi + \nabla\phi \cdot \mathbf{u}^e = 0,$$

where $\mathbf{u}^e$ is an extension of the velocity field $\mathbf{u}$ obtained from the surface PDE.

We present an algorithm to solve the system based on four main ingredients, namely

- a geometrically unfitted finite element method (TraceFEM) for the spatial discretization of the surface PDE,
- a narrow band DG method for solving the level set equation to track the surface evolution,
- a ghost penalty based extension method for the level set function, and
- a volume normal based extension method for the velocity field.

The extension methods for the level set and the velocity functions are needed since the surface PDE defines the velocity field only on the surface, but the level set equation is solved in a narrow band around the surface. In the talk, we describe these key components of the algorithm and present numerical results that demonstrate the performance and accuracy of the method.

Minisymposium M15

Iterative methods and preconditioners for (multiple) saddle point linear systems

Organisers

Luca Bergamaschi and Angeles Martinez

Eigenvalue bounds for symmetric multiple saddle-point matrices

Luca Bergamaschi *(University of Padova)* & Ángeles Martínez *(University of Trieste)* & John W. Pearson *University of Edinburgh)* & Andreas Potschka

(Clausthal University of Technology)

We develop eigenvalue bounds for symmetric multiple saddle-point linear systems, preconditioned with block diagonal preconditioners. We extend known results for 3×3 block systems [1] and for 4×4 systems [2] to an arbitrary number of blocks. Moreover, our results generalize the bounds in [3], developed for an arbitrary number of blocks, but with null diagonal blocks. Extension to the bounds when the Schur complements are approximated is also provided, using perturbation arguments. Practical bounds are also obtained for the double saddle-point linear system. Numerical experiments validate our findings.

References

[1] S. Bradley and C. Greif, *Eigenvalue bounds for double saddle-point systems*, IMA Journal of Numerical Analysis, 43 (2023), pp. 3564–3592.

[2] J. W. Pearson and A. Potschka, *On symmetric positive definite preconditioners for multiple saddle-point systems*, IMA Journal of Numerical Analysis, 44 (2024), pp. 1731–1750.

[3] J. Sogn and W. Zulehner, *Schur complement preconditioners for multiple saddle point problems of block tridiagonal form with application to optimization problems*, IMA Journal of Numerical Analysis, 39 (2018), pp. 1328–1359.

An H-Matrix Block Preconditioner for the RBF-FD discretized Oseen equations

Michael Koch & Sabine Le Borne *(TU Hamburg)*

The Radial Basis Function Finite Difference method (RBD-FD) is a meshless method for solving partial differential equations, that gained popularity in the last two decades. It provides an alternative to the Finite Element and Finite Difference method as it can provide high order of convergence as well as geometric flexibility. The application of the RBF-FD method to steady state fluid flow problems (e.g. Stokes or Oseen equations) poses some challenges for iterative solvers as the resulting saddle point systems are completely non-symmetric (even structurally non-symmetric) and there can be many non-zero entries per row (for high order discretizations).

In this talk we will briefly introduce RBF-FD method and discuss characteristics of the resulting saddle point matrix. Then we will present a block preconditioner which utilizes hierarchical matrices. We demonstrate the effectiveness of this preconditioner with some numerical results for the three-dimensional Oseen equations for challenging convection directions and domains.

Triangular preconditioners for double saddle point linear systems arising in the mixed form of poroelasticity equations

Ángeles Martínez *(University of Trieste)* & Luca Bergamaschi *(University of Padua)* & Massimiliano Ferronato *(University of Padua)*

This communication will analyze the spectral properties of the class of block triangular preconditioners developed in [2, 3] for the solution of the discrete stabilized mixed and mixed hybrid finite element formulation of Biot's poroelasticity equations. Biot's model couples Darcy's flow of a single-phase fluid with the quasi-static mechanical deformation of an elastic, fully saturated porous medium. In its mixed form, Darcy's law is explicitly considered as a governing equation along with the fluid mass balance, giving rise to the so-called three-field formulation, where the solid phase displacements, the pore fluid pressure, and Darcy's velocity are the independent unknown quantities. Biot's poroelasticity model is key in several relevant applications, ranging from geosciences, such as groundwater hydrology, geothermal energy extraction, and geological carbon and hydrogen storage problems to biomedicine. After discretization, a large double saddle point linear system must be iteratively solved. We have considered block triangular preconditioners based on both algebraic and physics-based approximations of the Schur complements. We have derived bounds on the eigenvalues of the corresponding preconditioned matrix, extending the results provided in [1], where a simpler case with the second and third diagonal blocks equal to zero is addressed. The results of numerical experiments show the quality of the theoretical bounds and illustrate the efficiency of the proposed preconditioners used with GMRES, especially in comparison with similar block diagonal preconditioning strategies along with the MINRES iteration. The efficiency of the proposed inexact preconditioners will be reported for large-size 3D realistic problems.

References

[1] F. Bakrani Balani, L. Bergamaschi, A. Martínez, and M. Hajarian, *Some preconditioning techniques for a class of double saddle point problems*, Numerical Linear Algebra with Applications, 31, e2551 (2024), pp. 1–22.

[2] M. Ferronato, M. Frigo, N. Castelletto, and J. A. White, *Efficient solvers for a stabilized three-field mixed formulation of poroelasticity*, Lecture Notes in Computational Science and Engineering, 139 (2021), p. 419 – 427.

[3] M. Frigo, N. Castelletto, M. Ferronato, and J. A. White, *Efficient solvers for hybridized three-field mixed finite element coupled poromechanics*, Computers and Mathematics with Applications, 91 (2021), p. 36 – 52.

Optimal and scalable augmented Lagrangian preconditioners for fictitious domain problems

Federica Mugnaioni *(Scuola Normale Superiore)* & Michele Benzi, Marco Feder, Luca Heltai

We present [1] preconditioning techniques for efficiently solving linear systems of equations with a block two-by-two [2] and three-by-three [3] structure arising from fictitious domain problems and from finite element discretizations of immersed boundary methods [4]. In particular, we propose two augmented Lagrangian-based preconditioners [5, 6] to accelerate the convergence of iterative solvers for these two classes of linear systems. We consider two relevant examples to illustrate the performance of these preconditioners when used in conjunction with flexible GMRES: the Poisson and the Stokes fictitious domain problems.

We provide a detailed spectral analysis of the proposed preconditioners, deriving lower and upper bounds for the eigenvalues of the preconditioned matrix and showing their independence with respect to discretization parameters. Furthermore, we discuss the eigenvalue distribution when inexact versions of the preconditioners are employed [7].

We show the effectiveness of the proposed approach and the robustness of our preconditioning strategies through extensive numerical tests in both two and three dimensions, using different immersed geometries. A key aspect of immersed methods is the interaction between non-matching meshes: the physical domain is embedded in a fixed background, enabling independent mesh generation but demanding careful treatment of coupling terms. The implementation of a suitable parallel solver is based on the C++ Finite Element library DEAL.II [8].

References

[1] M. Benzi, M. Feder, L. Heltai and F. Mugnaioni. Optimal and Scalable Augmented Lagrangian preconditioners for Fictitious Domain problems. *arXiv:2504.11339*, 2025

[2] M. Benzi, G. H. Golub and J. Liesen. Numerical solution of saddle point problems. *Acta Numerica*, 14:1–137, 2005.

[3] F. P. A. Beik and M. Benzi. Iterative methods for double saddle point systems. *SIAM Journal on Matrix Analysis and Applications*, 39(2):902–921, 2018.

[4] D. Boffi and L. Gastaldi. A fictitious domain approach with Lagrange multiplier for fluid-structure interactions. *Numer. Math.*, 135(3):711–732, 2017.

[5] M. Benzi and M. A. Olshanskii. An augmented Lagrangian-based approach to the Oseen problem. *SIAM Journal on Scientific Computing*, 28(6):2095–2113, 20006.

[6] F.P.A. Beik and M. Benzi. Preconditioning techniques for the coupled Stokes–Darcy problem: spectral and field-of-values analysis. *Numerische Mathematik*, 150(2):257–298, 2022

[7] F. Bakrani, L. Bergamaschi, A. Martinez and M. Hajarian. Some preconditioning techniques for a class of double saddle point problems. *Numerical Linear Algebra with Applications*, 31(4), e2551, 2024

[8] D. Arndt, W. Bangerth, M. Bergbauer, M. Feder, M. Fehling, J. Heinz, T. Heister, L. Heltai, M. Kronbichler, M. Maier, P. Munch, J.P. Pelteret, B. Turcksin, D. Wells, S. Zampini. The `deal.II` Library, Version 9.5. *Journal of Numerical Mathematics*, 31(3), pp. 231–246, 2023.

Preconditioners for Multiple Saddle-Point Systems and Applications to PDE-Constrained Optimization

John Pearson *(University of Edinburgh)* & Andreas Potschka

Optimization problems subject to PDE constraints form a mathematical tool that can be applied to a wide range of scientific processes, including fluid flow control, medical imaging, option pricing, biological and chemical processes, and electromagnetic inverse problems, to name a few. These problems involve minimizing a functional arising from some practical objective, while obeying a system of PDEs describing a scientific process. Of key interest is the numerical solution of the discretized linear systems arising from such problems, which motivates our focus on preconditioned iterative methods for these systems.

In particular, we describe recent advances in the preconditioning of multiple saddle-point systems, focusing on preconditioners which can be applied within MINRES, as these find considerable utility in solving such optimization problems as well as other applications. We extend the notion of block diagonal preconditioning to obtain a new class of block preconditioners which are also symmetric positive definite and lead (in the 'ideal' case) to an eigenvalue result independent of the number of blocks. This strategy provides a guaranteed convergence rate for MINRES, and often leads to superior convergence than block diagonal preconditioners in practice.

Time permitting, we may also discuss an inexact active-set method for large-scale nonlinear PDE-constrained optimization problems, coupled with block diagonal and block triangular preconditioners for multiple saddle-point systems which utilize suitable approximations for the relevant Schur complements.

MinAres and CAr: New Krylov methods for symmetric linear systems

Alexis Montoison *(Argonne National Laboratory)* & Dominique Orban *(Polytechnique Montréal)* & Michael Saunders *(Stanford University)*

We introduce a Krylov solver named MinAres for symmetric linear systems $Ax \approx b$, where A is possibly singular. MinAres is based on the symmetric Lanczos process, like Minres and Minres-QLP, but it minimizes $\|Ar_k\|$ in each Krylov subspace rather than $\|r_k\|$, where r_k is the current residual vector. In our experiments, MinAres terminates significantly earlier than Minres on ill-conditioned and singular linear systems.

We derive properties of MinAres from an equivalent solver named CAr, which is to MinAres as Cr is to Minres. CAr is not based on the Lanczos process and minimizes $\|Ar_k\|$ in the same Krylov subspaces as MinAres. We establish that MinAres and CAr generate monotonic $\|x_k - x^*\|$, $\|x_k - x^*\|_A$, and $\|r_k\|$ when A is positive definite.

MinAres and CAr are implemented in Julia as part of the package Krylov.jl. They are applicable to any floating-point system supported by Julia, including complex numbers, and can run on both CPUs and GPUs.

Minisymposium M16

Structure-preserving finite element methods

Organisers

Boris Andrews and Charles Parker

Designing conservative and accurately dissipative numerical integrators via auxiliary variables

Boris Andrews *(University of Oxford)* & Patrick Farrell *(University of Oxford & Charles University)*

Geometric numerical integrators are known to exhibit greater accuracy and physical reliability, in particular over long durations. However, there remain difficulties in devising schemes that conserve non-quadratic invariants or dissipation laws, in particular for systems of PDEs.

In this talk, we propose a framework for the construction of timestepping schemes that preserve dissipation laws and conserve multiple general invariants, via finite elements in time and the systematic introduction of auxiliary variables; each of these methods extends to arbitrary order in time. We demonstrate the ideas by constructing a novel energy-stable integrator for the Benjamin–Bona–Mahony equation.

Further novel applications of the framework will be discussed, including integrators that exactly conserve all
known invariants of general integrable systems, and finite-element schemes for the compressible Navier-Stokes equations that conserve mass, momentum, and energy, and provably possess non-decreasing entropy.

Structure-preserving approximation and error analysis for a viscoelastic phase separation model

Aaron Brunk & Mária Lukácová *(Johannes-Gutenberg University Mainz)*

Numerical methods for simulating transient systems that preserve underlying physical or geometric structures often demonstrate enhanced accuracy and reliability, particularly over long time intervals. Such methods are typically grounded in deep geometric principles and are especially effective for broad classes of problems, such as Hamiltonian or reversible systems. However, designing structure-preserving schemes for general equations remains a significant challenge—even when the system's structure is known. Moreover, conducting rigorous error analysis is even more difficult and typically only feasible for simplified problems.

In this talk, we consider a continuum dynamic model for viscoelastic phase separation. This model incorporates dynamic asymmetry between the two components, allowing it to capture additional morphologies that arise during the separation process. These morphologies cannot be described by the classical Model H, necessitating an extension to account for viscoelastic effects.

We propose a fully discrete approximation based on continuous Petrov-Galerkin methods in time and conforming finite element methods in space. The resulting discretization preserves key physical properties of the continuous system, namely mass conservation and energy dissipation. For a simplified version of the system—where the viscoelastic contribution to shear stress is neglected—we are also able to prove optimal error rates in both space and time using a relative energy framework.

Structure-preserving discretisation for the magneto-frictional equations in the Parker conjecture

Mingdong He *(University of Oxford)*, Patrick E. Farrell *(University of Oxford & Charles University)*, Kaibo Hu *(University of Edinburgh)* & Boris D. Andrews *(University of Oxford)*

The Parker conjecture, which explores whether magnetic fields in perfectly conducting plasmas can develop tangential discontinuities during magnetic relaxation, remains an open question in astrophysics. Helicity conservation provides a topological barrier during relaxation, preventing topologically nontrivial initial data relaxing to trivial solutions; preserving this mechanism discretely over long time periods is therefore crucial for numerical simulation. This work presents an energy- and helicity-preserving finite element discretization for the magneto-frictional system, for investigating the Parker conjecture. The algorithm preserves a discrete version of the topological barrier and a discrete Arnold inequality. We also discuss extensions to domains with nontrivial topology.

Finite element form-valued forms

Kaibo Hu *(University of Edinburgh)* & Ting Lin *(Peking University)*

We provide a finite element discretization of ℓ-form-valued k-forms on triangulation in nD for general k, ℓ and n and any polynomial degree. The construction generalizes finite element Whitney forms for the de Rham complex and their higher-order and distributional versions, the Regge finite elements and the Christiansen–Regge elasticity complex, the TDNNS element for symmetric stress tensors, the MCS element for traceless matrix fields, the Hellan–Herrmann–Johnson (HHJ) elements for biharmonic equations, and discrete divdiv and Hessian complexes in [Hu, Lin, and Zhang, 2025]. The construction discretizes the Bernstein–Gelfand–Gelfand (BGG) diagrams. Applications of the construction include discretization of strain and stress tensors in continuum mechanics and metric and curvature tensors in differential geometry

in any dimension.

Minisymposium M17

Numerical methods for optimization with PDE constraints
Organisers
Estefania Loayza Romero and John Pearson

Efficient Iterative Methods for the Solution of Sparse Tree-Coupled Saddle-Point Systems

Bernhard Heinzelreiter & Christoph Hansknecht & John W. Pearson & Andreas Potschka *(University of Edinburgh)*

A broad class of optimization problems with numerous applications involves sparsely connected optimization problems. These consist of a series of constrained subproblems linked through a relatively small subset of variables. Such problems play a crucial role in engineering applications, including stochastic programming, robust nonlinear model predictive control, and optimal control of networks (e.g., gas pipelines). Upon linearization and discretization, the problems reduce to the solution of linear sparse saddle-point systems, which mirror the tree-coupled structures. Depending on the application, the linear systems can reach regimes that black-box solvers cannot handle, requiring bespoke problem-specific solvers.

In this talk, we derive a suite of direct and (in particular) iterative solvers for saddle-point systems with a tree-coupled structure. Specifically, we extend well-studied structure-exploiting approaches for saddle-point systems by incorporating the graph-based coupling structure, where interactions between individual and otherwise isolated subsystems are expressed via generic coupling constraints. This allows us to make use of the special, sparse structure of the resulting Schur complement. We develop a range of preconditioners, which follow recursive and multi-level approaches. The majority of these methods are vastly parallelizable, allowing them to be applied in a real-time fashion. We prove a range of results relating to the convergence, complexity, and spectral properties of our algorithms. The performance of the preconditioners is demonstrated by applying them to a range of model problems. This includes model predictive control, multiple shooting for optimal control, and domain decomposition for PDE-constrained optimization problems. The numerical experiments validate our theoretical results and show improved performance over direct methods.

A Total Variation Flow Scheme for Ergodic Mean Field Games

Dante Kalise *(Imperial College London)* & Alessio Oliviero *(Sapienza University of Rome)* & Domènec Ruiz-Balet *(Université Paris-Dauphine)*

Motivated by recent developments in mean-field games in ecology, we establish a connection between the best response dynamics in evolutionary game theory, the minimization of the highest income of a game, and minimizing movement schemes. We develop a variational approach to compute solutions of first order ergodic mean-field games that may not possess an *a priori* variational structure. We present the construction of a JKO type method, its convergence, and different benchmarks.

A Riemannian Approach for PDE-Constrained Shape Optimization Using Outer Metrics

Estefania Loayza Romero & Lidiya Pryymak & Kathrin Welker *(University of Strathclyde)*

In PDE-constrained shape optimization, shapes are traditionally viewed as elements of a Riemannian manifold—-specifically as embeddings of the unit circle into the plane, modulo reparametrizations. The standard approach employs the Steklov-Poincaré metric to compute gradients for Riemannian optimization methods. A significant limitation of current methods is the absence of explicit expressions for the geodesic equations associated with this metric. Consequently, algorithms have relied on retractions (often equivalent to the perturbation of identity method in shape optimization) rather than true geodesic paths. Previous research suggests that incorporating geodesic equations, or better approximations thereof, can substantially enhance algorithmic performance. This talk presents numerical evidence demonstrating that using outer metrics—defined on the space of diffeomorphisms with known geodesic expressions—improves Riemannian gradient-based optimization by significantly reducing the number of required iterations and preserving mesh quality throughout the optimization process.

Fast iterative solvers for bilevel nonlocal denoising with NFFT kernels

Andrés Miniguano-Trujillo *(Maxwell Institute for Mathematical Sciences)* & John Pearson *(University of Edinburgh)*

In this talk, we revisit the bilevel optimisation framework for parameter learning in nonlocal image denoising models [1], with a specific focus on recent advancements in preconditioning strategies [2]. Building upon recent applications of the Nonequispaced Fast Fourier Transform (NFFT) [3] for efficient Gaussian kernel evaluation [4, 5,6], we focus on the structure and solution of the linear systems arising in the optimality conditions. We provide a spectral description of the nonlocal and unnormalised graph Laplacians. Then, we introduce a decomposition of the system through explicit and efficient transformations. Combining the deflation-inspired technique with the analysis of the numerical range of the system allows us to propose and analyse a family of dense preconditioners that can be applied in linear time to the decomposed system. As a result, we obtain nearly-constant conjugate gradient (CG) iterations for solving very ill-conditioned systems governed by scalings of the graph Laplacian in a matrix-free fashion. Numerical experiments demonstrate the scalability and robustness of the method across a range of images and noise levels.

Acknowledgements: Work supported by MACMIGS CDT Scholarship under EPSRC grant EP/ S023291/1.

References

[1] Marta D'Elia, Juan Carlos De Los Reyes, Andrés Miniguano-Trujillo. *Bilevel parameter learning for nonlocal image denoising models.* Journal of Mathematical Imaging and Vision 63, 753–775, 2021.

[2] Andrés Miniguano–Trujillo, John Pearson, Ben Goddard. *Efficient nonlocal linear image denoising: Bilevel optimization with Nonequispaced Fast Fourier Transform and matrix–free preconditioning* arXiv: 2407.06834, 2025.

[3] Jens Keiner, Stefan Kunis, Daniel Potts. *Using NNFT 3 - a software library for various nonequispaced fast Fourier transforms.* ACM Transactions on Mathematical Software 36, 1–30, 2009.

[4] Franziska Nestler, Martin Stoll, Theresa Wagner. *Learning in high-dimensional feature spaces using ANOVA-based fast matrix-vector multiplication.* Foundations of Data Science 4(3), 423-440, 2022.

[5] Theresa Wagner, John Pearson, Martin Stoll. *A preconditioned interior point method for support vector machines using an ANOVA-decomposition and NFFT-based matrix–vector products.* arXiv: 2312.00538, arXiv, 2023.

[6] Franziska Nestler, Martin Stoll, Theresa Wagner. *Fast evaluation of additive kernels: feature arrangement, Fourier methods, and kernel derivatives* arXiv: 2404.17344, arXiv, 2024.

Shape optimization on various Riemannian shape spaces

Kathrin Welker & Estefania Loayza-Romero & Lidiya Pryymak & Tim Suchan *(Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg)*

Shape optimization is concerned with identifying shapes (or subsets of $\mathbb{R}^n$, $n \in \mathbb{N}$) behaving in an optimal way with respect to a given physical system. It has been an active field of research for the past decades and is used for example in engineering. Many relevant problems in the area of shape optimization involve a constraint in the form of a partial differential equation (PDE). Theory and algorithms in shape optimization can be based on techniques from differential geometry, e.g., a Riemannian manifold structure can be used to define the distances of two shapes. Thus, shape spaces are of particular interest in shape optimization. In this talk, we apply the differential-geometric structure of Riemannian shape spaces to the theory of classical PDE-constrained shape optimization. We have a look on inner and outer Riemannian metrics, different Riemannian shape spaces and present algorithms to solve PDE-constrained shape optimization problems.

Geometry Denoising with Preferred Normal Vectors

Manuel Weiss & Lukas Baumgärtner & Ronny Bergmann & Roland Herzog & Stephan Schmidt *(IWR Heidelberg)*

Mesh denoising and segmentation are fundamental tasks in computer graphics, often complicated by noise and irregular geometry. In this talk, I will present our recent work on variational methods for tackling these challenges, coupling a smooth fidelity term based on shape priors with total variation (TV) regularization. We focus on a specific problem setting where the mesh is assumed to align with a prescribed set of normal directions. This fits naturally into the framework of variational methods, where a mesh denoising and an assignment problem are solved simultaneously. We demonstrate how it can be efficiently solved using an Alternating Direction Method of Multipliers (ADMM) approach. Finally, we explore extensions of this framework to handle more complex scenarios, including the incorporation of underlying partial differential equations (PDEs).

Thinking in parallel: Preconditioning variational time-dependent mean field games

Heidi Wolles Ljósheim *(University of Edinburgh)*, Dante Kalise *(Imperial College London)*, John W. Pearson *(University of Edinburgh)*, Francisco J. Silva *(Université de Limoges)*

Mean field games have received a lot of attention in recent years as they provide a powerful framework for modelling the strategic behaviour of a large number of interacting agents. However, even the well-behaved (variational) ones require careful numerical approximation. A promising approach is to discretise the system of PDEs and treat one set of the equations as constraints in an optimisation problem. Employing finite differences, we solve the resulting finite-dimensional convex optimisation problem using the Chambolle-Pock primal–dual algorithm. As this involves computing proximal operators and solving ill-conditioned linear systems at each iteration, we propose a general class of parallel-in-time preconditioners based on diagonalization techniques using discrete Fourier transforms. These enable efficient, scalable iterative solvers with robustness across a wide range of viscosities. We further develop fast solvers for the resulting ill-conditioned systems arising at each time step, using exact recursive schemes for structured grids while allowing for other geometries. Numerical experiments confirm the improved performance and parallel scalability of our approach.

Multi-level Nonlinear Optimal Control with Neural Surrogate Models

Dante Kalise *(Imperial College London)*, Estefania Loayza-Romero *(University of Strathclyde)*, Kirsten A. Morris *(University of Waterloo)*, **Zhengang Zhong** *(University of Warwick)*

Optimal actuator and control design is studied as a multi-level optimization problem, where the actuator design is evaluated based on the performance of the associated optimal control. The evaluation of the optimal control for a given actuator realisation is a computationally demanding task, for which the use of a neural network surrogate is proposed. The use of neural network surrogates to replace the lower level of the optimization hierarchy enables the use of fast gradient-based and gradient-free consensus-based optimization methods to determine the optimal actuator design. Through further study of the optimality conditions, we enhance the surrogate model leveraging Sobolev training, allowing for scenarios with limited training data. The effectiveness of the proposed surrogate models and optimization methods is assessed in tests related to optimal actuator location for heat and Burger's equation control.

Minisymposium M18

Numerical methods for fractional-derivative problems

Organisers

Natalia Kopteva and Yubin Yan

Optimal quadrature for Marchaud derivatives and integral fractional Laplacians

Yanghong Huang *(University of Manchester)*

Numerical evaluation of fractional-type derivatives are usually challenging due to the presence of singularities. In this talk, optimal quadrature rule are proposed for Marchaud derivatives $\int_0^\infty (f(x) - f(x+t))\, t^{-1-\alpha} dt$ and integral fractional Laplacians $\int_0^\infty (2f(x) - f(x+t) - f(x-t)) t^{-1-\alpha} dt$. When f is smooth and decays fast at infinity, the main difficulty in obtaining a consistent order of accuracy near the singularity is resolved by making the rule exact only for lower order polynomials essentially present in the integrand (without the factor $t^{-1-\alpha}$). The new quadrature rules improve the accuracy near the singularity, while maintaining the expected order of convergence away from it.

Pointwise-in-time error bounds for a fractional-derivative parabolic problem on quasi-graded meshes

Seán Kelly & Natalia Kopteva *(University of Limerick)*

An initial-boundary value, quasi-linear subdiffusion problem involving a Caputo time derivative of fractional order $\alpha \in (0,1)$ is considered. The solutions of which typically exhibit a singular behaviour at initial time. Building on the framework of Kopteva and Meng [1] for analyzing L1-type discretization errors on graded and uniform temporal meshes, we relax the regularity assumptions on the solution. Specifically, we assume $|\delta_t^l u(\cdot,t)| \lesssim 1 + t^{\sigma-l}$ for some $\sigma \in (0,1) \cup (1,2)$ and any $l = 0, 1, 2$, thus accommodating a broader class of solution behaviors. Under this more general assumption on the solution, we give sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading (including uniform meshes, also considered by Li, Qin, and Zhang [2]. We also refine the stability result derived in [1] to allow a more general grading parameter. Extensions to the cases with non-smooth initial conditions

will also be considered.

References

[1] N. Kopteva and X. Meng: Error Analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions. SIAM J. Numer. Anal., 58, (2020).

[2] D. Li, H. Qin, and J. Zhang: Sharp pointwise-in-time error estimate of L1 scheme for nonlinear subdiffusion equations J. Comput. Math., 42 (2024).

Pointwise-in-time error estimates for time-fractional semilinear and quasilinear parabolic equations

Natalia Kopteva & Seán Kelly *(University of Limerick)*

For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0,1)$, we give sharp pointwise-in-time error bounds in the spatial L_2 and L_∞ norms on graded temporal meshes with arbitrary degree of grading. The purpose of this talk will be to show that the error analysis framework developed in [1, 2, 3] seamlessly extends to the semilinear case [4, 5], as well as to the quasilinear case (the latter being more recent joint work with Sean Kelly).

References

[1] N. Kopteva, Error analysis of the L1 method on graded and uniform meshes for a fractional-derivative problem in two and three dimensions, Math. Comp., 88 (2019), 2135–2155.

[2] N. Kopteva and X. Meng, Error analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions, SIAM J. Numer. Anal., 58 (2020), 1217–1238.

[3] N. Kopteva Error analysis of an L2-type method on graded meshes for a fractional-order parabolic problem, Math. Comp., 90 (2021), 19–40.

[4] N. Kopteva, Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions, SIAM J. Numer. Anal., 58 (2020), 2212–2234.

[5] N. Kopteva, Error analysis of an L2-type method on graded meshes for semilinear subdiffusion equations, Appl. Math. Lett., 160 (2025), 109306.

***hp*-FEM for the integral fractional Laplacian: quadrature**

Jens Markus Melenk & Björn Bahr & Markus Faustmann (*TU Wien*)

For the Dirichlet problem of the integral fractional Laplacian on intervals Ω and on polygons Ω, it has recently been shown that exponential convergence of the *hp*-FEM based on suitably designed meshes can be achieved, [2]. These meshes are geometrically refined towards the edges and corners of Ω. The geometric refinement towards the edges results in anisotropic meshes away from corners. The use of such anisotropic elements is crucial for the exponential convergence result. These mesh design principles are the same ones as those for *hp*-FEM discretizations of the Dirichlet spectral fractional Laplacian in polygons, for which [1] recently established exponential convergence.

In this talk, we address the issue of setting the stiffness matrix. We show that a judicious combination of Duffy-like transformations and hp-quadrature techniques allow one to set up the matrix with work growing algebraically in the problem size while retaining the exponential convergence of *hp*-FEM. The emphasis will be placed on the 1D fractional Laplacian, [4].

References

[1] Lehel Banjai, Jens M. Melenk, and Christoph Schwab. Exponential convergence of *hp* FEM for spectral fractional diffusion in polygons. *Numer. Math.*, 153(1):1–47, 2023.

[2] M. Faustmann, C. Marcati, J.M. Melenk, and Ch. Schwab. Exponential convergence of *hp*-FEM for the integral fractional Laplacian in polygons. *SIAM J. Numer. Anal.*, 61:2601–2622, 2023.

[3] Markus Faustmann, Carlo Marcati, Jens Markus Melenk, and Christoph Schwab. Weighted Analytic Regularity for the Integral Fractional Laplacian in Polygons. *SIAM J. Math. Anal.*, 54(6):6323–6357, 2022.

[4] Björn Bahr, Markus Faustmann, Jens Markus Melenk. an Implementation of *hp*-FEM for the fractional

Laplacian, *Comput. Math. Appl.* 176:324–348, 2024

Numerical analysis of fractional diffusion equations with boundary effects

Ercília Sousa *(University of Coimbra)*

Fractional diffusion equations, associated with Lévy processes, model anomalous diffusive transport in various physical systems. When boundary conditions are present, they significantly influence the numerical formulation of these problems. We examine both Dirichlet and reflecting boundary conditions, emphasizing their impact on the numerical approach. Due to the non-local nature of these equations, Neumann type problems can arise in different ways, depending on how reflections of external jumps are defined. We propose numerical methods to solve these diffusive models and demonstrate how the presence of boundaries changes the general structure of the problem and of the numerical method. In the end, we analyze the influence of different boundary conditions on the solutions.

Correction of a high-order numerical method for approximating time-fractional wave equation

Yubin Yan *(University of Chester)*

A high-order time discretization scheme to approximate the time-fractional wave equation with the Caputo fractional derivative of order $\alpha \in (1, 2)$ is studied. We establish a high-order formula for approximating the Caputo fractional derivative of order $\alpha \in (1, 2)$. Based on this approximation, we propose a novel numerical method to solve the time-fractional wave equation. Remarkably, this method corrects only one starting step and demonstrates second-order convergence in both homogeneous and inhomogeneous cases, regardless of whether the data is smooth or nonsmooth. We also analyze the stability region associated with the proposed numerical method. Some numerical examples are given to elucidate the convergence analysis.

This is a joint work with M. Ramezani and R. Mokhtari

Minisymposium M19

Advances in Linear Algebra and Preconditioners

Organisers

Ann Paterson and Razan Abu-Labdeh

Preconditioning for high-frequency time-harmonic waves with directional sweeping

Niall Bootland & Tyrone Rees *(STFC Rutherford Appleton Laboratory)*

We consider the potential for parallelism within an approach to precondition problems involving high-frequency time-harmonic waves. We take inspiration from domain decomposition strategies known as sweeping methods, which have gained notable interest for their ability to yield nearly-linear asymptotic complexity and which can also be favourable for high-frequency problems. While successful approaches exist, such as those based on higher-order interface conditions, perfectly matched layers (PMLs), or complex tracking of wave fronts, they can often be quite involved or tricky to implement. We investigate here the use of simple sweeping techniques applied in different directions and the potential for using sweeps in parallel within the solver. We further link to similar features in very high-frequency applications within ptychography using a simplified time-harmonic forward model.

Conjugate Direction Methods Under Inconsistent Systems

Alexander Lim & **Yang Liu** *(University of Oxford)* & Fred Roosta

Since the 1950s, the conjugate gradient (CG) and conjugate residual (CR) methods have been central to solving positive definite linear systems.

Since their inception, these methods have been extended beyond positive definite to indefinite, albeit consistent, settings. Going one step further, we investigate the theoretical and empirical properties of these methods under inconsistent systems. Among other things, we show that small modifications to the original algorithms allow for the pseudo-inverse solution. Furthermore, we show that CR is essentially equivalent to MINRES, proposed by Paige and Saunders in 1975, in such contexts.

Lastly, we conduct a series of numerical experiments to shed lights on their numerical stability (or lack thereof) and their performance for inconsistent sys-

tems. we also demonstrate that, unlike CR and contrary to popular belief, CG can exhibit significant numerical instability, bordering on catastrophe in some instances.

A Low-Rank Tensor approach for Local Refinement in IGA

Tom-Christian Riemer & Martin Stoll *(Technische Universität Chemnitz)*

Local refinement is a key strategy for improving the efficiency and accuracy of numerical simulations, particularly when fine resolution is only needed in localized regions. Isogeometric Analysis (IGA) offers a unified framework where both the computational domain and the solution fields are represented using the same basis functions, typically B-splines or NURBS. To enable local refinement within IGA, truncated hierarchical B-splines (THB-splines) have been introduced in [1], preserving the partition of unity while reducing the support of the basis functions, which leads to sparser system matrices and tensors.

In this talk, we present a novel low-rank method for the efficient assembly of mass and stiffness tensors when the solution is approximated using THB-splines. Building on an additive heuristic for level-wise assembly [2], we introduce a greedy strategy that identifies a small set of local tensor-product structures among the refined cells and basis functions, yielding a compact low-rank representation. To perform efficient integration, we apply the weight function interpolation presented in [3] with the alternating minimal energy (AMEn) solver [4], reducing the multidimensional quadrature to univariate operations. This approach mitigates memory consumption and computational cost, especially in high-dimensional problems. Although not universally applicable, it is particularly effective when refinement regions remain relatively simple. Preliminary numerical experiments using MATLAB and the GeoPDEs toolbox validate the potential of our method to alleviate computational bottlenecks in adaptive isogeometric simulations.

References

[1] C. Giannelli, B. Jüttler, H. Speleers, THB-splines: The truncated basis for hierarchical splines, Computer Aided Geometric Design, Volume 29, Issue 7, 2012, Pages 485-498, ISSN 0167-8396, https://doi.org/10.1016/j.cagd.2012.03.025.

[2] E. M. Garau, R. Vázquez, Algorithms for the implementation of adaptive isogeometric methods using hierarchical B-splines, Applied Numerical Mathematics, Volume 123, 2018, Pages 58-87, ISSN 0168-9274, https://doi.org/10.1016/j.apnum.2017.08.006.

[3] A. Bünger, S. Dolgov, M. Stoll, A Low-Rank Tensor Method for PDE-Constrained Optimization with Isogeometric Analysis, SIAM Journal on Scientific Computing, 42, 1, A140-A161, 2020, https://doi.org/10.1137/18M1227238.

[4] S. V. Dolgov, D. V. Savostyanov, Alternating Minimal Energy Methods for Linear Systems in Higher Dimensions, SIAM Journal on Scientific Computing, 36, 5, A2248-A2271, 2014, https://doi.org/10.1137/140953289.

Convergence Behavior of GMRES on Tridiagonal Toeplitz Systems

Fei Chen & Kirk M. Soodhalter *(Trinity College Dublin)*

Discretizing PDEs leads to linear systems with large, sparse coefficient matrices. When linear, constant-coefficient PDEs with Dirichlet boundary conditions are discretized on uniform meshes, one can obtain Toeplitz, multilevel Toeplitz and/or block Toeplitz systems [1, 2]. Toeplitz matrices have constant diagonals, and multilevel and block Toeplitz matrices have related structures, that can be exploited to speed up GMRES, and aid convergence analysis. Such systems are widely solved by Krylov subspace methods.

Let

$$Ax = b, \tag{1}$$

where the matrix A is Toeplitz, b is a known right-hand side, and x is the unknown solution. GMRES starts with an initial guess, x_0, and select $x_k, k = 1, 2, \cdots$, such that $x_k - x_0 \in \mathcal{K}_k(A, r_0)$:=span $\{r_0, Ar_0, \cdots, A^{(k-1)}r_0\}$, where $r_0 = A(x - x_0)$.

For a symmetric system, the convergence behavior of MINRES, which is mathematically equivalent to GMRES for a symmetric system, can usually be characterized by the eigenvalues and the RHS. However, when A is nonsymmetric, GMRES convergence behavior is much more complicated to describe; in extreme cases, the spectrum bears no relation to the convergence rate. In [4], the authors prove that any non-increasing convergence curve is possible for GMRES by constructing a linear system of prescribed nonzero eigenvalues with a given convergence curve.

In spite of the difficulties, there has been plenty of work in the literature inspecting the convergence behavior of GMRES. For instance, in [5], the authors point out that, for a general nonsingular matrix A, the convergence behavior of GMRES is related to the

distribution of eigenvalues of A, and provide an upper bound. However, each eigenvalue is either treated as a member of some cluster, or an outlier to any cluster. For the cases where eigenvalues are not spreading out far away from each other, for example, those of a tridiagonal Toeplitz matrix, or when the clusters are far away from each other, one fails to find a meaningful upper bound since it becomes too loose. In [6], Meurant shows through APS parametrization [7] of A that GMRES could have different convergence behaviors for two different matrices with the same spectrum. Nevertheless, a reconstructed matrix A in this case does not preserve the Toeplitz structure in general. As for tridiagonal matrix systems, Liesen and Strakoš analyze the convergence behavior of GMRES when $|\alpha| \approx |\beta| \gg |\gamma|$ [8]. For a more general case where $\beta| \neq |\gamma|$, Li and Zhang provide upper bounds and asymptotic speeds of the 2-norm of the k^{th} residual via Chebyshev polynomial of the first kind [9] and the second kind [10]. Through our experiments, we find that given the same tridiagonal Toeplitz matrix and different right hand sides, almost all of GMRES convergence curves are much closer to the worse curve, i.e. the upper bound provided in [9] and [10]. In our work, we formulate equations based on APS parametrization of A with the constraint that each diagonal is constant to explore what convergence regimes are possible for a tridiagonal Toeplitz system.

Without loss of generality, we assume the main diagonal of the matrix A is 1,

$$A = \begin{bmatrix} 1 & \gamma & 0 & \cdots & 0 \\ \beta & 1 & \gamma & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \beta & 1 & \gamma \\ 0 & 0 & 0 & \beta & 1 \end{bmatrix} \in \mathbb{R}^{n\times n}, \qquad (2)$$

where β and $\gamma \in \mathbb{R}$.

Let $K = [b|Ab|\cdots|A^{n-1}b]$ be the Krylov matrix. Let $r_j, j = 1, \cdots, n-1$, be the residual at iteration j of GMRES applied to the Toeplitz system, and $h = (\eta_1, \cdots, \eta_n)^T$, where $\eta_j = \sqrt{r_{j-1}^2 - r_j^2}, j = 1, \cdots, n$, with $j_n \equiv 0$. The unique QR factorization of the Krylov residual matrix $B := AK$ is $B = WR$, where W is orthonormal and R is upper triangular. The uniqueness is determined through $b = Wh$; see [7]. Authors of [7] show that one can assign a sequence of positive nonincreasing values to $r_j's$ and construct a pair of matrix A and right hand side b such that the residual of the j^{th} iteration of GMRES is $r_j, j = 1, \cdots, n$. Since h appears to be directly linked with W, we attempt to analyze GMRES convergence behavior through W and the construction of the related tridiagonal Toeplitz matrices and corresponding right hand sides. We show that for any orthonormal matrix $W \in \mathbb{R}^{3\times 3}$, we can generate different pairs of tridiagonal Toeplitz matrix A and a corresponding right hand side b through the upper triangular matrix R. We also explore the possibility to construct such pairs given any orthonormal matrix W of an arbitrary size and whether it is possible to construct two different pairs of $A's$ and $b's$ such that they share the same h.

References

[1] C. Garoni and S. Serra-Capizzano, *Generalized Locally Toeplitz Sequences: Theory and Applications*, vol. I Springer Cham, 2017.

[2] C. Garoni and S. Serra-Capizzano, *Generalized Locally Toeplitz Sequences: Theory and Applications*, vol. II Springer Cham, 2018.

[3] A. Greenbaum, V. Pták, Z. Strakoš, *Any non increasing convergence curve is possible for GM-RES*, SIAM J. Matrix Anal. Appl., vol 17 (1996), No.3, 465–469.

[4] S.L. Campbell, I.C.F. Ipsen, C.T. Kelley and C.D. Meyer, *GMRES and the minimal polynomial*, BIT Numerical Mathematics, vol 36(1996), no.4, 664–675.

[5] G. Meurant, *GMRES and the Arioli, Pták and Strakoš parametrization*, BIT Numerical Mathematics, vol 52(2012), 687–702.

[6] M. Arioli, V. Pták and Z. Strakoš, *Krylov sequences of maximal length and convergence of GMRES*, BIT Numerical Mathematics, vol 38(1998) 636–643.

[7] J. Liesen and Z. Strakoš, *Convergence of GMRES for tridiagonal Toeplitz matrices*, SIAM J. Matrix Anal. Appl., vol 26(2004), no.1, 233–251.

[8] R.C. Li and W. Zhang, *The rate of convergence of GMRES on a tridiagonal Toeplitz linear system*, Numerische Mathematik, vol. 112(2009), 267–293.

[9] R.C. Li and W. Zhang, *The rate of convergence of GMRES on a tridiagonal Toeplitz linear system II*, Linear Algebra and its Applications, vol 12(2009), 2425–2436.

Filtration of Lanczos vectors in hybrid CG Tikhonov iteration

Kirk M. Soodhalter *(Trinity College Dublin)* & Daniel Gerth *(Technische Universität Chemnitz)* (formerly)

We consider iterative methods for solving a linear ill-posed problem of the form $Ax \approx y = y^\delta - \delta \cdot n$ wherein $A : \mathcal{X} \to \mathcal{Y}$ is a compact linear operator, and y^δ is a version of the right-hand side obtained by noisy measurements, with $\|n\| = 1$ and $0 < \delta \ll 1$. We assume that we only have access to y^δ. It is well known that naïve solution using the pseudoinverse operator $A^\dagger y^\delta$ may lead to amplification of the measurement noise, unbounded in the infinite-dimensional case and bounded but large in the finite-dimensional case.

Conjugate gradients applied to the normal equations (CG) $A^*Ax^\delta = A^*y^\delta$ with an appropriate stopping rule and CG applied to the system solving for a Tikhonov-regularized solution (CGT) $(A^*A+cI_\mathcal{X})x^{(\delta,c)} = A^*y^\delta$ ($c > 0$ is the Tikhonov parameter) are closely related methods. It has been long observed that they build iterates from the same family of Krylov subspaces, due to the scalar shift invariance property of Krylov subspaces [4]; i.e., $\mathcal{K}_m(A^*A, A^*y^\delta) = \mathcal{K}_m(A^*A + cI_\mathcal{X}, A^*y^\delta)$. One can express both CG-based iterates with respect to the same Lanczos basis. In particular, one can use this to understand how the representation of the CGT iterates change as a function of c with $c \to 0$ yielding a CG iterate. Let $x_m^\delta = \sum_{i=1}^m z_i^{(m)} v_i$ be the CG iterate where $\{v_i\}_{i=1}^m$ is the Lanczos basis for $\mathcal{K}_m(A^*A, A^*y^\delta)$. One can show that the CGT iterate can be expressed as $x_m^{(\delta,c)} = \sum_{i=1}^m \gamma_i^{(m)}(c) z_i^{(m)} v_i$, where $\left\{\gamma_i^{(m)}(c)\right\}_{i=1}^m$ are functions of the Tikhonov parameter.

These coefficient multiplier functions can be shown to have decay properties as $c \to \infty$ with the speed of decay increasing with i, asymptotically. This has the effect of filtering out the contribution of the later terms of the CG iterate. Thus, we call these functions *Lanczos filters*, as they express the effect of CGT regularization in terms of the CG expressed in the Lanczos basis rather than in terms of the singular vector basis, as is the case of classical definition of filter function in regularization theory [3]. We build upon the work in [1] to frame it all correctly in the context of infinite dimensional ill-posed problems. These ideas build on [6, 5] in finite dimensions.

We demonstrate with numerical experiments that good parameter choices correspond to appropriate damping of the Lanczos vectors corresponding to larger amplifications of the measurement noise. One could consider approaches other than Tikhonov for damping amplified noise. We conclude by noting that analysis of other hybrid regularization schemes via damping of subspace basis vectors from the iteration itself may be a useful avenue for understanding the behavior of these methods for different choice of parameter, etc.

References

[1] A. Alqahtani, R. Ramlau, and L. Reichel 2022.

[2] J. Chung and S. Gazzola 2024.

[3] H. W. Engl, M. Hanke, and A. Neubauer 1996.

[4] A. Frommer and P. Maass 1999.

[5] I. Hnětynková, M. Kubínová, and M. Plešinger 2017.

[6] I. Hnětynková, M. Plešinger, and Z. Strakoš 2009.

GMRES upper bound based on $\epsilon-$pseudospectra for preconditioned Toeplitz systems

Razan Abu-Labdeh & Jennifer Pestana *(University of Strathclyde)*

PDE models typically require numerical discretisation with sufficiently fine meshes to capture solution features, transforming the problem into solving one or more systems of linear equations, $Ax = b$. Due to several factors, these systems are often large and nonsymmetric and highly nonnormal. Krylov subspace methods, such as GMRES, are powerful tools for solving these sparse systems, but preconditioning is usually required to increase efficiency. While descriptive convergence theory exists to guide preconditioner choice when A is normal, it is less informative for nonnormal ones. Due to the nonnormality, GMRES bounds based on eigenvalues, the field of values and pseudospectra can fail to be descriptive [1].

Our work aims to also utilise the underlying PDE and discretisation properties to better understand the GMRES convergence. We show that in many instances preconditioned (multilevel) Toeplitz and non-Toeplitz problems, which typically belong to generalized locally Toeplitz (GLT) matrix sequences [2], can often be decomposed into the identity plus a low-rank perturbation and a small-norm perturbation, resulting in an eigenvalue clustering near 1 with a few outliers. We characterise the pseudospectra in this case, and present a new GMRES bound that takes into account the outlier in a way that overcomes overestimations seen in other bounds.

References

[1] Mark Embree, How descriptive are GMRES convergence bounds?, arXiv preprint *arXiv:2209.01231*, 2022.

[2] Carlo Garoni, Stefano Serra-Capizzano, Generalized locally Toeplitz sequences: theory and applications, volume 1, *Springer*, 2017.

Minisymposium M20

Numerical methods for nonlinear dispersive and wave Equations

Organisers

Buyang Li and Katharina Schratz

Computing rough solutions of the KdV equation below L^2

Jiachuan Cao *(Karlsruhe Institute of Technology)*, Buyang Li, Yifei Wu & Fangyan Yao

We establish a novel numerical and analytical framework for solving the Korteweg–de Vries (KdV) equation in the negative Sobolev spaces, where classical numerical methods fail due to their reliance on high regularity and inability to control nonlinear interactions at low regularities. Numerical analysis is established by combining a continuous reformulation of the numerical scheme, the Bourgain-space estimates for the continuous reformulation, and a rescaling strategy that reduces the reformulated problem to a small initial value problem, which allow us to bridge a critical gap between numerical analysis and theoretical well-posedness by designing the first numerical method capable of solving the KdV equation in the negative Sobolev spaces. The numerical scheme is proved to have nearly optimal-order convergence with respect to the spatial degrees of freedom in the $H^{-\frac{1}{2}}$ norm for initial data in H^s, with $-\frac{1}{2} < s \leq 0$, a result unattainable by existing numerical methods.

Efficient simulation of wave propagation via low-rank approximation

Daniel Appelö *(Virginia Tech)*, Andreas Granath *(Umeå University)* & **Siyang Wang** *(Umeå University)*

We consider underwater acoustic wave propagation in the frequency domain modelled by the Helmholtz equation. A major challenge in solving this equation numerically lies in the high spatial resolution required and the indefiniteness of the discretised system, particularly at high frequencies. To address these difficulties, we employ the WaveHoltz iterative method, which reformulates the problem as a time-dependent wave equation with time-periodic forcing. We discretise the wave equation in space by an efficient finite difference method satisfying a summation-by-parts property, ensuring stability and high-order accuracy. By utilising the intrinsic structure of the solution in the considered application, we develop a low-rank approximation strategy in the time-dependent wave solver. By compressing the solution space, we achieve substantial reduction in computational cost and memory usage of solving 2D and 3D Helmholtz problems.

Enhanced Higher-Order Multiscale Method for the Wave Equation

Balaje Kalyanaraman *(Umea University)* & **Felix Krumbiegel** *(Karlsruhe Institute of Technology)* & Roland Maier *(Karlsruhe Institute of Technology)* & Siyang Wang *(Umea University)*

Modeling waves in highly oscillatory media using standard methods comes at high computational costs as the oscillations need to be resolved. In this talk we propose a numerical homogenization strategy based on the higher-order localized orthogonal decomposition method that enriches coarse finite element functions such that convergence can be obtained even when the fine-scale features are not resolved. The higher-order convergence can be shown for very general bounded PDE coefficients that require minimal assumptions. We give an ideal construction of the enriched basis with a suitable localization strategy and present numerical examples to confirm the theoretical findings.

An Explicit Filtered Lie Splitting Scheme for the Original Zakharov System with Low Regularity Error Estimates in All Dimensions

Hang Li *(Sorbonne University)* & Lun Ji *(AMSS, Chinese Academy of Sciences & University of Innsbruck)* & Chunmei SU *(Tsinghua University)*

In this talk, we present an error estimate for the filtered Lie splitting scheme applied to the Zakharov system, characterized by solutions exhibiting very low regularity across all dimensions. Our findings are derived from the application of multilinear estimates established within the framework of discrete Bourgain spaces. Specifically, we demonstrate that when the solution $(E, z, z_t) \in H^{s+r+1/2} \times H^{s+r} \times H^{s+r-1}$, the error in $H^{r+1/2} \times H^r \times H^{r-1}$ is $\mathcal{O}(\tau^{s/2})$ for $s \in (0, 2]$, where $r = \max(0, \frac{d}{2} - 1)$. To the best of our knowledge, this represents the first explicit error estimate for the splitting method based on the original Zakharov system, as well as the first instance where low regularity error estimates for coupled equations have been considered within the Bourgain framework. Furthermore, numerical experiments confirm the validity of

our theoretical results.

Convergence of a moving window method for the Schrödinger equation with potential on R^d

Arieh Iserles & Buyang Li & **Fangyan Yao** *(Hong Kong Polytechnic University)*

We propose a novel framework, called moving window method, for solving the linear Schrödinger equation with an external potential in R^d. This method employs a smooth cut-off function to truncate the equation from Cauchy boundary conditions in the whole space to a bounded window of scaled torus, which is itself moving with the solution. This allows for the application of established schemes on this scaled torus to design algorithms for the whole-space problem. Rigorous analysis of the error in approximating the whole-space solution by numerical solutions on a bounded window is established. Additionally, analytical tools for periodic cases are used to rigorously estimate the error of these whole-space algorithms. By integrating the proposed framework with a classical first-order exponential integrator on the scaled torus, we demonstrate that the proposed scheme achieves first-order convergence in time and $\gamma/2$-order convergence in space for initial data in $H^\gamma(R^d) \cap L^2(R^d; |x|^{2\gamma} dx)$ with $\gamma \geq 2$. In the case where $\gamma = 1$, the numerical scheme is shown to have half-order convergence under an additional CFL condition. In practice, we can dynamically adjust the window when waves reach its boundary, allowing for continued computation beyond the initial window. Extensive numerical examples are presented to support the theoretical analysis and demonstrate the effectiveness of the proposed method.

Minisymposium M21

Quantum Numerical Algorithms
Organisers
Subhayan Roy Moulik and Pranav Singh

Fault-tolerant quantum simulation of generalized Hubbard models

Nick Blunt *(Riverlane)* & Andreas Juul Bay-Smidt, Frederik Ravn Klausen, Christoph Sünderhauf, Róbert Izsák, Gemma C. Solomon

Simulating quantum systems of interacting electrons is a widely investigated use case for quantum computers. Despite significant optimization efforts, the quantum simulation of challenging systems such as the FeMoco complex and cytochrome P450 have been estimated to require at least millions of physical qubits and billions of Toffoli gates, which is far beyond the capabilities of near-term devices. Recently, it has been shown that fault-tolerant simulation of classically non-trivial Hubbard model instances may be possible with around one million Toffoli gates. Therefore, there is the exciting possibility that such model systems may be relevant in the "early fault-tolerant" regime. However, these previous studies have focused on the square-lattice Hubbard model. In this talk, we will present an efficient method to perform quantum simulation of generalized Hubbard models, for arbitrary lattices and Hamiltonians with long-range interactions, including extended Hubbard models and model Hamiltonians used in chemistry, such as the PPP model. We will give an introduction to Trotterization for quantum simulation, and present our scheme, which we call Tile Trotterization. We will discuss the use of Tile Trotterization in quantum phase estimation, and compare our results to qubitisation, which is a current state-of-the-art approach. We show that our scheme has better scaling with system size than qubitisation, and can be performed with low T gate counts. To conclude, we will discuss the potential use of this technique on early fault-tolerant quantum computers, and the considerations that this will involve.

Quantum algorithms for the exponential of Hamiltonian matrices

Guannan Chen *(University of Bath)*, Subhayan Roy Moulik *(University of Cambridge)*, Pranav Singh *(University of Bath)*

Computing the time evolution of quantum systems, by solving the Schrödinger equation and approximating matrix exponentials, is a fundamental task in quantum computing and numerical analysis. In this talk, we discuss some techniques for Hamiltonian simulation on quantum computers, including rational approximations, variational methods, and exponential splittings, with a focus on enabling long time steps that allow practical implementation on near-term quantum devices.

On Convergence and Efficiency of Quantum Imaginary Time Evolution

Tobias Hartung *(Northeastern University London)* & Karl Jansen *(DESY, Zeuthen)*

Many current applications of quantum simulations are based on variational methods. These variational methods are commonly subject to effects that can prevent convergence to global solutions. While options to circumvent these obstacles exist, they generally come at the cost of efficiency.

In this talk, we will consider the quantum imaginary time evolution. We will show convergence guarantees for imaginary time evolution to the global optimum, and prove convergence rates as well as the absence of critical slowing down. This will allow us to obtain estimates on the evolution time required to reach fidelity thresholds. In particular, for combinatorial optimization problems we can conclude that success probability thresholds can be reached in linear evolution time with respect to system size in qubits and the inverse energy gap.

Furthermore, we will discuss the circuit compilation for quantum imaginary time evolution in detail. Considering bounded order systems with polynomial coefficient scaling in particular, we will show that the corresponding quantum circuits implementing imaginary time evolution can be compiled using polynomial resources in qubits, inverse energy gap, and approximation error bounds.

Hybrid Classical and Quantum Deep Learning

Catherine Higham *(University of Glasgow)*

Hybrid deep learning promises greater efficiency by combining classical optimization algorithms with quantum circuits and algorithms. In this talk I will discuss work [1] that transfers classically trained neural nets to a quantum annealer for faster classification. I will also outline recent work exploring classical/quantum variational algorithms for risk estimation.

References

[1] Higham, C. F. and Bedford, A. (2023) Quantum deep learning by sampling neural nets with a quantum annealer. Scientific Reports, 13, 3939.

Selected results on quantum numerical algorithms at Quantinuum

Conor McKeever *(Quantinuum)*

I present a selection of our work at Quantinuum that relates to quantum numerical algorithms. Specifically, I focus on the experimental realization of quantum singular value transformation on Quantinuum's quantum computers, in the context of quantum many-body Hamiltonian simulation [1] and ground-state preparation [2].

References

[1] Y. Kikuchi et al., "Realization of quantum signal processing on a noisy quantum computer", npj Quantum Inf. 9, 93 (2023).

[2] E. Karacan et al., "Filter-enhanced adiabatic quantum computing on a digital quantum processor", arXiv:2503.20674 [quant-ph].

Discovering a compiler for a quantum device

E. Babson *(University of California, Davis)* & S. Roy Moulik *(University of Cambridge)*

A device takes in finite sequences of gates from a short list and returns Y or N with some probabilities. The protocol has three phases. First there is the discovery phase in which runs are chosen to build a classical compiler for the device. Second with the compiler in hand any long string of gates is replaced with a short one for which the device produces similar probabilities. Finally the short string is run on the device.

The class of devices for which we analyse this protocol work by starting with a fixed state represented in some vector space on which each gate acts linearly and after running the input string of gates applies a fixed linear effect to get a real number which is the probability of returning Y. We will further assume compactness and a weak mixing condition. Our analysis will be couched in the parameters v the dimension of the state space, g the dimension of the compact closure of the group generated by the gates, l the length of long words and c^{-1} the probability that the compiler is incorrect for some long word.

The device gives a continuous function from G to [0,1] as the probabilities of Y for nearby words and devices with the same functions will be considered similar. We find a regime with large state space but small group for which this compilation is efficient while learning and storing classically the entire device is not.

Quantum dimension reduction for stochastic simulation

Thomas J. Elliott (*University of Manchester*)

Simulating quantum dynamics on a classical computer bears a resource cost that grows exponentially with the size of the system, and even the simplest of quantum systems often exhibit seemingly complex behaviours. This apparent problem can be recast as a positive – complex classical systems may be efficiently simulated on simple quantum computers. In this talk I will discuss the application of quantum technologies to the modelling of stochastic processes, for which quantum simulators can operate with lower memory dimension than any classical alternative – i.e., a *quantum dimension reduction*. I will highlight

examples of quantitative scaling divergences in modelling highly non-Markovian processes, wherein the provably-memory-minimal classical simulator must store diverging amounts of information with increasing precision, while arbitrary precision can be achieved with a finite-sized quantum simulator. I will further describe how lossy quantum dimension reduction can be used for high fidelity, low memory cost stochastic simulation in settings where no exact quantum dimension reduction is possible. I will also discuss recent work on the experimental implementation of such quantum dimension reduction.

Minisymposium M22

Advancements and applications of solvers for PDE systems with nonsmooth structures

Organisers
Ioannis Papadopoulos and Michael Hintermüller

A Descent Algorithm for the Optimal Control of ReLU Neural Network Informed PDEs Based on Approximate Directional Derivatives

Michael Hintermüller *(Weierstrass Institute Berlin)* & G. Dong *(Central South University, China)*, and K. Papafitsoros *(Queen Mary University London)*

We propose and analyze a numerical algorithm for solving a class of optimal control problems for learning-informed semilinear partial differential equations (PDEs). Such PDEs contain constituents that are in principle unknown and are approximated by nonsmooth ReLU neural networks. We first show that direct smoothing of the ReLU network with the aim of using classical numerical solvers can have disadvantages, such as potentially introducing multiple solutions for the corresponding PDE. This motivates us to devise a numerical algorithm that treats directly the nonsmooth optimal control problem, by employing a descent algorithm inspired by a bundle-free method. Several numerical examples are provided and the efficiency of the algorithm is shown.

Semi-smooth Newton methods for mappings between nonlinear spaces

Anton Schiela & Laura Weigl *(Universität Bayreuth)*

An important class of nonlinear PDEs can be formulated as variational problems on nonlinear spaces, such as Hilbert manifolds. To solve these problems efficiently, also in the presence of non-smoothness, a semi-smooth Newton method can be applied. In this talk we will extend the notion of semi-smoothness to mappings between nonlinear manifolds and present a geometric version of this concept for the case of variational problems, which can be formulated via mappings from a manifold into a dual vector bundle. To render Newton steps well defined in this setting, we have to equip the vector bundle with a connection. We will discuss local convergence and provide some numerical examples.

The latent variable proximal point algorithm for variational problems with inequality constraints

Ioannis Papadopoulos *(Weierstrass Institute)* & Jørgen Dokken, Patrick Farrell, Brendan Keith, Thomas Surowiec

The latent variable proximal point (LVPP) algorithm is a framework for solving infinite-dimensional variational problems with pointwise inequality constraints. The algorithm is a saddle point reformulation of the Bregman proximal point algorithm. Although equivalent at the continuous level, the saddle point formulation is significantly more robust after discretization.

LVPP yields simple-to-implement numerical methods with robust convergence and observed mesh-independence for obstacle problems, contact, fracture, plasticity, and others besides; in many cases, for the first time. The framework also extends to more complex constraints, providing means to enforce convexity in the Monge–Ampère equation and handling quasi-variational inequalities, where the underlying constraint depends implicitly on the unknown solution. Moreover the algorithm is largely discretization agnostic allowing one to discretize with very-high-order *hp*-finite element methods in an efficient manner. In this talk, we will describe the LVPP algorithm in a general form and apply it to a number problems from across mathematics.

Preprint: https://arxiv.org/abs/2503.05672.

A Nitsche method for fluid flow with set-valued slip boundary conditions

Alexei Gazca & Franz Gmeineder & Erika Maringová-Kokavcova & Tabea Tscherpel *(Charles University Prague)*

The classical no-slip (or homogeneous Dirichlet) boundary condition for fluid flow is not appropriate in many situations, as fluids will often slip at solid walls. In this work we propose a theoretical framework that is able to capture a wide variety of slip models, includ-

ing linear (Navier) slip, non-linear (and possibly non-smooth) slip described by coercive monotone graphs, and non-monotone slip. A finite element scheme is proposed, in which the non-penetrability condition at the wall is enforced with a Nitsche formulation. Numerical experiments implemented in firedrake will also be presented.

The theoretical framework captures also non-coercive and dynamic (i.e. including a time derivative) slip boundary conditions. For this we refer to the talk by T. Tscherpel.

Numerical approximation of an optimal insulation problem defined on a polyhedral domain

Alex Kaltenbach *(Technical University of Berlin)* & Harbir Antil (George Mason University) & Keegan L. A. Kirk (George Mason University)

In this talk, we are interested in the numerical approximation of a both non-local and non-smooth convex minimization problem that allows to determine the optimal distribution, given by $h\colon \partial\Omega \to [0, +\infty)$, of a given amount $m \in \mathbb{N}$ of insulating material attached to the boundary $\partial\Omega$ of a thermally conducting body $\Omega \subseteq \mathbb{R}^d$, $d \in \mathbb{N}$. The non-local and non-smooth convex minimization problem is obtained as a model reduction (in the sense of Γ-convergence) of an extension of the physical setting in the work on the *'thin insulation'* case by Buttazzo (*cf.* [1] to polyhedral domains.

In order to tackle the non-local and non-smooth character of the problem, we resort to a (Fenchel) duality framework:
(a) At the continuous level, using (Fenchel) duality relations, we derive an *a posteriori* error identity that can handle arbitrary admissible approximations of the primal and dual formulations of the non-local and non-smooth convex minimization problem;
(b) At the discrete level, using discrete (Fenchel) duality relations, we derive an *a priori* error identity that applies to a Crouzeix–Raviart discretization of the primal formulation and a Raviart–Thomas discretization of the dual formulation. The proposed framework leads to error decay rates that are optimal with respect to the specific regularity of a minimizer. Since the discrete dual formulation can be written as a quadratic program, it is solved using a primal-dual active set strategy interpreted as semi-smooth Newton scheme. Then, a solution of the discrete primal formulation is reconstructed from the solution of the discrete dual formulation by means of an inverse generalized Marini formula.

References

[1] G. Buttazzo. Thin insulation layers: the optimization point of view. In *Material Instabilities in Continuum Mechanics: Related Mathematical Problems: the Proceedings of a Symposium Year on Material Instabilities in Continuum Mechanics*, pages 11–19. Oxford University Press, USA, 1988.

A Simple Introduction to the SiMPL Method for Density-Based Topology Optimization

Dohyun Kim & Boyan S. Lazarov & Thomas M. Surowiec & Brendan Keith *(Brown University)*

We present a novel first-order algorithm for density-based topology optimization: Sigmoidal Mirror descent with a Projected Latent variable (SiMPL). SiMPL combines three key ideas: (i) entropy-induced Bregman geometry for handling bound constraints, (ii) a projected latent variable formulation to ensure feasibility of iterates at every iteration, and (iii) adaptive line search strategies with guaranteed monotonicity.

Designed to balance mathematical rigor and engineering efficiency, SiMPL leverages the geometry induced by the (negative) Fermi–Dirac entropy to define a Bregman divergence tailored to bound constraints on the density. We take the first optimize and then discretize approach to topology optimization yielding a mesh- and order-independent algorithm. One of the novel approach is to use a projected latent variable to represent the density, which allows us to avoid realizing the density in the polynomial space. This not only simplifies the algorithm but also provides a natural extension to higher-order finite elements. In addition, we suggests two backtracking line searches with approximated Lipschitz-like initial step size. Combined with adaptive step size, the method produces a monotonically decreasing sequence of objective function values. In this talk we will present the algorithm and its convergence analysis, and demonstrate its performance on a variety of topology optimization problems, including compliance minimization and compliant mechanism.

Optimization of Total Variation-Regularized Functions using Inexact Proximal Solves in Hilbert Space

Robert J. Baraldi & Drew P. Kouri *(Sandia National Laboratories)*

Total Variation (TV) optimization penalizes the gradient of a control variable or state; such regularization has found utility in image processing, inverse problems, and topology optimization. We will address two fundamental challenges with TV optimization: (i) the

typical slow convergence of existing TV optimization methods; and (ii) the inexact evaluation of the TV proximity-operator. The proximal operator of the TV function can be just as difficult as solving the original problem. We allow for inexact proximal subproblem solves with an error-tolerance governed by a trust-region globalization scheme. We propose an algorithm for general nonsmooth, nonconvex TV optimization and illustrate our technique on imaging and topology problems.

Higher-order bounds-preserving methods for time-dependent partial differential equations via variational inequalities

John Stephens & Robert Kirby & Daniel Shapero *(Baylor University)*

The solutions to partial differential equations frequently satisfy bounds constraints. When using finite element or finite difference methods, if one wishes to construct an approximate solution that satisfies these same bounds, great care is required. In a finite element context, one can replace a discrete variational problem with a discrete variational inequality. This allows for the selection of an approximate solution from a set of functions which satisfy the bounds constraints. Solving nonlinear optimization problems, though incurring a practical expense, bypasses known order barriers for linear problems and allows for the possibility of high-order and uniformly bounds-constrained finite element methods.

It is difficult to work with the entire set of bounds-constrained polynomials. However, the polynomials whose coefficients, when represented in the Bernstein basis, satisfy the bounds constraints form a convenient subset with which to work. Selecting an approximation from this set via a variational inequality, one obtains an approximation which is uniformly bounds-constrained, independent of the mesh used. Recent work seeks to extend this approach to collocation-type Runge-Kutta methods. Using a stage-value formulation, the collocating polynomial can be cast in the Bernstein basis to enforce bounds constraints uniformly in time. Examples are shown in which optimal order accuracy is observed.

A neural network approach to learning solutions of a class of elliptic variational inequalities

Clemens Sirotenko & Amal Alphonse & Michael Hintermüller *(Weierstrass Institute)* & Alexander Kister *(BAM)* and Chin Hang Lun (*Tripadvisor UK)*

In this talk, we will present a novel weak adversarial framework for solving obstacle problems using neural networks. By reformulating the problem via (generalised) regularised gap functions into a natural min-max structure, we create a setting well suited to learning-based approaches. We will outline the error analysis, highlighting both discretisation and statistical errors. Then, we will explain how parametrising the solution and test functions as neural networks allows us to solve the resulting min-max problem using a modified gradient descent-ascent method. Numerical experiments illustrate the robustness of the method. We will conclude by discussing current limitations, open problems, and future challenges of the approach.

Minisymposium M23

Approximating complex systems: Surrogates, reduced order modelling and dimension reduction

Organisers
Elliot Addy, Benjamin M Kent and Aretha Treckentrup

Lengthscale-informed sparse grids for high dimensional Gaussian process emulation

Elliot Addy & Jonas Latz & Aretha Teckentrup *(University of Edinburgh)*

Gaussian process emulation is a widely used approach to surrogate modelling, in which the aim is to cheaply approximate outputs of computer models whilst also keeping track of the uncertainty in these predictions. Emulators, however, fall prey to the curse of dimensionality, prompting extensive research into the design of efficient experiments for high-dimensional settings. For functions in certain mixed Sobolev spaces, sparse grid designs have demonstrated improved convergence rates that scale only logarithmically with the input dimension. Yet, for large dimensions ($d > 10$), these methods still quickly become computationally prohibitive. In this work, we propose a novel sparse grid construction that is adapted to the lengthscale parameter in Matérn-type kernels. For functions exhibiting sufficient anisotropy, this construction allows for scalable emulation in arbitrarily high dimensions, while relying on weaker regularity assumptions than existing anisotropic approaches.

Dimensionality reduction and learning for optimization problems

Coralia Cartis *(University of Oxford)*

We discuss various ways of improving scalability and

performance of optimisation algorithms that are particularly applicable when special structure is present in the objective, such as low-rank. We explore linear (and time permitting nonlinear) embeddings that make use of various levels of problem information (none, zero-, first- and second-order) to generate the embeddings. Time permitting, both local and global optimization methods will be addressed.

Sketch In, Sketch Out: Accelerating both Learning and Inference for Structured Prediction with Kernels

Tamim El Ahmad & Luc Brogat-Motte & Pierre Laforgue & Florence d'Alché-Buc *(University of Edinburgh)*

Leveraging the kernel trick in both the input and output spaces, surrogate kernel methods are a flexible and theoretically grounded solution to structured output prediction. If they provide state-of-the-art performance on complex data sets of moderate size (e.g., in chemoinformatics), these approaches however fail to scale. We propose to equip surrogate kernel methods with sketching-based approximations, applied to both the input and output feature maps. We prove excess risk bounds on the original structured prediction problem, showing how to attain close-to-optimal rates with a reduced sketch size that depends on the eigendecay of the input/output covariance operators. From a computational perspective, we show that the two approximations have distinct but complementary impacts: sketching the input kernel mostly reduces training time, while sketching the output kernel decreases the inference time. Empirically, our approach is shown to scale, achieving state-of-the-art performance on benchmark data sets where non-sketched methods are intractable.

Multi-Index Stochastic Collocation for PDEs with Imperfect Solvers

Benjamin M. Kent & Lorenzo Tamellini & Matteo Giacomini & Antonio Huerta *(CNR-IMATI, Pavia)*

This talk considers the construction of surrogate models for parametric partial differential equations (PDEs) using Multi-Index Stochastic Collocation (MISC). In some settings, in addition to standard solver error, the PDE approximations used to build a MISC response surface are affected by solver "noise" (e.g. due to iterative methods, time-stepping,...). This type of solver error is particularly problematic in low fidelity models and may be parameter-dependent and hard to estimate and control a priori. This noise is interpolated by MISC and can corrupt the approximated response surface, often observed as spurious high-frequency oscillations, and spoils any subsequent uncertainty quantification analysis.

We propose an improved version of MISC that can detect such phenomena. In our updated adaptive algorithm, at each iteration, we inspect the spectral content of the response for each fidelity. If the decay of their spectral polynomial coefficients stagnates due to the solver noise the fidelity is subsequently ignored at the refinement stage.

Numerical experiments show the effectiveness of our approach in preventing corruption of the MISC approximation.

Reduced Basis Methods for Computing Stochastic Galerkin Surrogates

Catherine E. Powell *(University of Manchester)*

Stochastic Galerkin (SG) methods provide a surrogate modelling technique for facilitating forward UQ in PDEs with uncertain inputs. Unlike conventional sampling methods, such as Monte Carlo, SG schemes yield approximations which are functions of the random input variables so that all realisations of the PDE solution are effectively approximated simultaneously. Since they use simple tensor product approximation spaces, standard SG schemes give rise to huge linear systems with coefficient matrices with a characteristic Kronecker product structure. Solving these systems is often a bottleneck when working on standard desktop computers.

A potential remedy is to recast the Kronecker product linear systems as multi-term matrix equations and to consider solving these using adaptive low rank methods that iteratively construct a reduced basis and apply projection techniques to solve a problem of reduced size. While the strategy has proved effective for symmetric and positive definite problems arising from simple model problems (i.e, elliptic PDEs with random diffusion coefficients), is it less clear how such reduced basis methods can be optimally designed for other classes of problems, such as those of saddle point type. In this talk, we will discuss such issues and assess the feasibility of accelerating the construction of SG surrogates using reduced basis matrix equation solvers for elasticity and poroelasticity problems.

Nonlinear reduction model for solving parameterized PDE problems using machine learning techniques

Jingye Li & Jinglai Li & Alex Bespalov *(University of Birmingham)*

In many real-world engineering systems, solving parameterized partial differential equations (PDEs) over a large set of parameter values is inevitable. Reduced order modelling (ROM) is a popular technique that replaces the full-order model by a reduced model with much smaller dimension. Linear ROMs obtained using, e.g., reduced basis methods are likely to perform poorly when the Kolmogorov n-width of a solution manifold decays slowly. To address this issue, we propose a new method that consists of two stages: first, finding a low-dimensional space and second, constructing a nonlinear map from the low-dimensional space to a high-fidelity solution space using a feed-forward neural network. Thus, we build a surrogate model using two local nonlinear operators. The first operator is the same for all parameter values and maps from the space spanned by the reduced basis to a low-dimensional space. The second operator is parameter dependent and maps the low-dimensional space to the solution space. In this talk, we discuss the above solution strategy and apply it to some parameterized PDEs for which standard linear ROMs do not perform well. The results of numerical experiments show that the proposed approach significantly improves the accuracy in approximating PDE solutions compared to standard linear ROMs. Furthermore, the nonlinear operator that constructs a low-dimensional representation of the solution manifold in the first stage of the method also improves the training efficiency of the neural network in the second stage. These advantages make our computational strategy suitable for fast simulations using parameterized PDEs, where expensive multiple solves are required for different input parameters.

Minisymposium M24

Recent Advances in Numerical Linear Algebra

Organisers

Françoise Tisseur and Zhengbo Zhou

BTOAR: The Two-Level Orthogonal Arnoldi Procedure

Michael Jones *(University of Manchester)*

The TOAR (Two-Level Orthogonal Arnoldi) method is an Arnoldi-like method for computing a few dominant eigenpairs of a large, sparse quadratic eigenvalue problem (QEP). It generates an orthonormal basis for a *second order* Krylov subspace and uses it to project the large, sparse QEP onto said subspace, producing a small, dense QEP that can be solved fully. Block versions of the standard Arnoldi algorithm exist and are used in practice. They are able to exploit higher-level BLAS routines and are supposed to be better at computing non-simple (or clustered) eigenvalues. This talk explores the extension of the TOAR method to block form.

Computing Accurate Eigenvalues using the Preconditioned Jacobi Algorithm

Nicholas J. Higham, Françoise Tisseur, Marcus Webb & **Zhengbo Zhou** *(University of Manchester)*

We propose a mixed-precision Jacobi algorithm that uses low precision to compute the preconditioner, applies it in high precision, and solves the preconditioned eigenproblem using the cyclic Jacobi algorithm in working precision. Our rounding error analysis yields meaningfully smaller relative forward error bounds for the computed eigenvalues compared to those of the Jacobi algorithm without preconditioning. Furthermore, we prove that, after preconditioning, if the off-diagonal entries of the preconditioned matrix are sufficiently small relative to its smallest diagonal entry, the relative forward error bound becomes independent of the condition number of the original input matrix. We also provide two constructions for the preconditioner that exploit low precision.

A Fast BB Reduced Minimization Algorithm for Nonnegative Viscosity Optimization in Optimal Damping

Qingna Li & Françoise Tisseur *(Beijing Institute of Technology) & (University of Manchester)*

In this paper, we consider the fast optimization algorithm for optimal viscosities in damping system. Different from standard models that minimize the trace of the solution of parameterized Lyapunov equation, the nonnegative constraints for viscosities are added in the optimization model, which hasn't been considered before. To solve the new model, a new algorithm is then proposed, aiming at reducing the residuals of the corresponding KKT conditions. By combining with the Barzilai-Borwein stepsize, the proposed BB residual minimization algorithm (short for BBRMA) can further speed up to deal with large scale linear vibration systems. Extensive numerical results verify the high efficiency of the proposed algorithm.

Error Analysis of Matrix Multiplication with Narrow Range Floating-Point Arithmetic

Mantas Mikaitis & Theo Mary *(University of Leeds)*

High-performance computing hardware now supports

many different floating-point formats, from 64 bits to only 4 bits. While the effects of reducing precision in numerical linear algebra computations have been extensively studied, some of these low precision formats also possess a very narrow range of representable values, meaning underflow and overflow are very likely. The goal of this article is to analyze the consequences of this narrow range on the accuracy of matrix multiplication. We describe a simple scaling that can prevent overflow while minimizing underflow. We carry out an error analysis to bound the underflow errors and show that they should remain dominated by the rounding errors in most practical scenarios. We also show that this conclusion remains true when multiword arithmetic is used. We perform extensive numerical experiments that confirm that the narrow range of low precision arithmetics should not significantly affect the accuracy of matrix multiplication—provided a suitable scaling is used.

Updating Katz centrality in complex networks by counting walks

Francesca Arrigo & Daniele Bertaccini & Alessandro Filippo *(University of Strathclyde)*

Katz centrality is one of the most popular walk-based centrality indices in network science, with applications spanning from identification of potential disease genes in protein-interaction networks to the optimization of artificial neural networks.

Introduced in 1953, it builds on the simple observation that the powers of the adjacency matrix A of a graph can be used to count traversals in a network, and on the intuition that longer walks should carry less importance then longer ones when defining a measure of importance, or centrality, for nodes. More specifically, *Katz centrality of node i* is defined as the ith entry of the vector

$$\sum_{r=0}^{\infty} \alpha^r A^r \mathbf{1}, \qquad \alpha > 0,$$

where $\mathbf{1}$ is the vector of all ones. Whenever $\alpha\rho(A) < 1$, with $\rho(A)$ the spectral radius of A, the above converges to the matrix function $(I-\alpha A)^{-1}$ and computing Katz centrality reduces to solving a sparse linear system.

Since 1953, the size of networks for which computing Katz centrality is useful has grown exponentially. Moreover, the networks we interact with on a day-to-day basis change in time; roads get disrupted and users delete social media accounts. Solving a linear system from scratch every time one such change happens is computationally expensive. Strategies like the Sherman-Morrison-Woodbury formula are also impractical, as they require diagonal elements of $(I-\alpha A)^{-1}$, which we do not usually have access to.

In this talk we discuss the problem of approximately updating Katz centrality scores after nodes or edges are removed from the network. The approach we take in this talk is purely combinatoric and it is based on new results that allow to exactly count walks that visit a certain set of entities (nodes or edges) in the graph. We will describe two algorithms that update Katz centrality after node/edge removal using $O(m)$ operations, where m is the number of undirected edges in the original graph. Numerical experiments to support our theoretical findings will also be discussed, in particular highlighting that our methods outperform standard linear solvers, even when these are fed the original vector of centralities as their initial guess.

References

[1] F. Arrigo, D. Bertaccini, and A. Filippo. "Updating Katz centrality by counting walks." *arXiv preprint arXiv:2411.19560* (2024).

Generalizing Reduced Rank Extrapolation to Low-Rank Matrix Sequences

Pascal Boef & Patrick Kürschner & Xiaobo Liu & Joseph Maubach & Jens Saak & Wil Schilders & **Jonas Schulze** *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)* & Nathan van den Wouw

Reduced rank extrapolation (RRE) is an acceleration method typically used to accelerate the iterative solution of nonlinear systems of equations using a fixed-point process. In this context, the iterates are vectors generated from a fixed-point mapping function. However, when considering the iterative solution of large-scale matrix equations, the iterates are low-rank matrices generated from a fixed-point process for which, generally, the mapping function changes in each iteration. To enable acceleration of the iterative solution for these problems, we propose two novel generalizations of RRE. First, we show how to effectively compute RRE for sequences of low-rank matrices. Second, we derive a formulation of RRE that is suitable for fixed-point processes for which the mapping function changes each iteration. We demonstrate the potential of the methods on several numerical examples involving the iterative solution of large-scale Lyapunov and

Riccati matrix equations.

Eigenvalue backward errors of Rosenbrock systems and related optimization problems

Ding Lu, **Anshul Prajapati**, Punit Sharma, & Shreemayee Bora *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)*

Consider the *Rosenbrock system matrix* (also known as the Rosenbrock system polynomial) in the standard form

$$S(s) = \begin{bmatrix} A - sI_r & B \\ C & P(s) \end{bmatrix}, \tag{1}$$

where $s \in \mathbb{C}$, $A \in \mathbb{C}^{r,r}$, $B \in \mathbb{C}^{r,n}, C \in \mathbb{C}^{n,r}$, I_r is an identity matrix of size r, and $P(s)$ is a matrix polynomial of degree d given by $P(s) = \sum_{j=0}^{d} s^j A_j$ with $A_j \in \mathbb{C}^{n,n}$ for $j = 0, \ldots, d$. We assume $S(s)$ is *regular*, i.e., $\det(S(s)) \neq 0$ for some $s \in \mathbb{C}$, and call a scalar $\lambda \in \mathbb{C}$ an eigenvalue of $S(s)$ if $\det(S(\lambda)) = 0$. The Rosenbrock system matrix (1) and its associated eigenvalues are of fundamental importance in the field of linear system theory. It is well-known that the dynamical behaviour of a linear time-invariant system in the form of

$$\Sigma: \quad \begin{cases} \dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + P(\frac{d}{dt})u(t) \end{cases} \tag{2}$$

can be analyzed through the system matrix $S(s)$ in (1), as it contains the information on the *poles and zeros* of the transfer function of Σ, which determines the stability and performance of the system. The eigenvalues of $S(s)$ are known as the *invariant zeros* of Σ and can be used to recover the zeros of the system. For more details, refer to [1].

The eigenvalue backward error for matrix polynomials have been widely studied in the literature. A recurring theme in those studies is the preservation of particular structure within the perturbation matrices, such as symmetry, skew-symmetry, and sparsity. However, these works have not yet addressed the unique block structure in the Rosenbrock system matrix $S(s)$ given by (1).

We address the problem of computing the eigenvalue backward error of the Rosenbrock system matrix under various types of block perturbations, taking into account both full and partial perturbations across its four component blocks: A, B, C, and $P(s)$. We establish novel characterizations of these backward errors using a class of minimization problems involving the Sum of Two generalized Rayleigh Quotients (SRQ2). For computational purposes and analysis, we reformulate such optimization problems as minimization of a rational function over the joint numerical range of three Hermitian matrices. This reformulation eliminates certain local minimizers of the original SRQ2 minimization and allows for convenient visualization of the solution. Furthermore, by exploiting the convexity within the joint numerical range, we derive a characterization of the optimal solution using a Nonlinear Eigenvalue Problem with eigenvector dependency (NEPv). Our numerical experiments demonstrate the benefits and effectiveness of the NEPv approach for SRQ2 minimization in computing eigenvalue backward errors of Rosenbrock systems.

References

[1] H. H. Rosenbrock. State-space and Multivariable Theory. *Thomas Nelson and Sons*, London, 1970.

[2] D. Lu, A. Prajapati, P. Sharma, and S. Bora. Eigenvalue backward errors of Rosenbrock systems and optimization of sums of Rayleigh quotients. To appear in *SIAM Journal on Matrix Analysis and Applications*, 2025.

Approximating large-scale Hessian matrices using secant equations

Jaroslav M. Fowkes & Nicholas I. M. Gould *(STFC Rutherford Appleton Laboratory)* & Jennifer A. Scott *(STFC Rutherford Appleton Laboratory and University of Reading)*

Large-scale optimization algorithms frequently require sparse Hessian matrices that are not readily available. Existing methods for approximating large sparse Hessian matrices either do not impose sparsity or are computationally prohibitive. To try and overcome these limitations, we propose a novel approach that seeks to satisfy as many componentwise secant equations as necessary to define each row of the Hessian matrix. A naive application of this approach is prohibitively expensive on Hessian matrices that have some relatively dense rows, but by carefully taking into account the symmetry and connectivity of the Hessian matrix we are able devise an approximation algorithm that is fast and efficient with scope for parallelism. Example sparse Hessian matrices from the CUTEst test problem collection for optimization illustrate the effectiveness and robustness of our proposed method.

Deflation Strategies for Nonlinear Eigenvalue Problems

Françoise Tisseur *(The University of Manchester)*

Deflation for linear eigenvalue problems is a standard technique that consists of removing a known eigenvalue or changing it so that the other eigenvalues are

easier to find. In this talk we discuss and compare different strategies to deflate eigenvalues of nonlinear eigenvalue problems. We will pay particular attention to the quadratic eigenvalue problem, describe a structural engineering application where deflation is needed, and introduce a deflation strategy based on structure preserving transformations.

Minisymposium M25

Numerical Analysis and AI
Organisers
Alexander Bastounis, Des Higham and Marcelo Pereyra

On the consistent reasoning paradox of intelligence and optimal trust in AI: The power of 'I don't know'

Alexander Bastounis *(King's College London)*

We introduce the Consistent Reasoning Paradox (CRP). Consistent reasoning, which lies at the core of human intelligence, is the ability to handle tasks that are equivalent, yet described by different sentences ('Tell me the time!' and 'What is the time?'). The CRP asserts that consistent reasoning implies fallibility, in particular, human-like intelligence in AI necessarily comes with human-like fallibility. Specifically, it states that there are problems, e.g. in basic arithmetic, where any AI that always answers and strives to mimic human intelligence by reasoning consistently will hallucinate (produce wrong, yet plausible answers) infinitely often. The paradox is that there exists a non-consistently reasoning AI (which therefore cannot be on the level of human intelligence) that will be correct on the same set of problems. The CRP also shows that detecting these hallucinations, even in a probabilistic sense, is strictly harder than solving the original problems, and that there are problems that an AI may answer correctly, but it cannot provide a correct logical explanation for how it arrived at the answer. Therefore, the CRP implies that any trustworthy AI (i.e., an AI that never answers incorrectly) that is also consistently reasoning must be able to say 'I don't know'. Moreover, this can only be done by implicitly computing a new concept that we introduce, termed the 'I don't know' function – something currently lacking in modern AI. In view of these insights, the CRP also provides a glimpse into the behaviour of Artificial Superintelligence (ASI). An ASI cannot be 'almost sure', nor can it always explain itself, and therefore to be trustworthy it must be able to say 'I don't know'.

Deceptive Diffusion: Attacking with Generative AI

Desmond J. Higham, *(University of Edinburgh)* & Lucas Beerens *(University of Edinburgh)* & Catherine Higham *(University of Glasgow)*

I will introduce the concept of deceptive diffusion—training a generative AI model on attacked data so that it directly produces images that fool a classifier. Whereas traditional adversarial attack algorithms perturb an existing image to induce a misclassification, a deceptive diffusion model can create an arbitrary number of new, misclassified images that are not associated with training or test images. As well as revealing AI vulnerabilities, deceptive diffusion offers the possibility of strengthening defence algorithms by providing adversarial training data at scale, including types of misclassification that are otherwise difficult to find.

Neural Network Surrogates for Bayesian Inverse Problems

Christian Jimenez Beltran, Antonio Vergari, Aretha Teckentrup & Konstantinos Zygalakis *(University of Edinburgh)*

Inverse problems associated with differential equations are central to numerous scientific and engineering applications, where we often need to estimate model parameters from noisy or incomplete data. Traditional numerical methods for solving these problems can be computationally expensive, particularly when computing the likelihood in a Bayesian framework, as this requires the evaluation of a forward model. In this talk, I will explore the potential of neural networks as surrogates to address these challenges. I will begin by reviewing an algorithm that trains neural networks to approximate parametric differential equations. Then, I will present a novel method that incorporates Laplace Approximation, enabling efficient approximation of the forward model while providing reliable uncertainty estimates. By comparing this approach with traditional methods, I will demonstrate how it significantly reduces computational costs while maintaining accurate posterior approximations. I will also show experimental results and compare our method to Gaussian Process regression. These findings underscore the promise of neural networks as reliable and scalable tools for solving inverse problems in complex

systems.

Inexpensive adversarial attacks on image classifiers

Aizhan Issagali & Desmond Higham *(University of Edinburgh)*

Convolutional neural networks are known to be vulnerable to adversarial attacks - an imperceptible perturbation to an image can cause a change in classification. Standard attack algorithms use explicit or approximate gradient information; partial derivative with respect to the input data. We will explore the possibility of using less expensive alternatives.

Bayesian computation with generative diffusion models by Multilevel Monte Carlo

Abdul-Lateef Haji-Ali & Marcelo Pereyra *(Heriot-Watt University)* & Luke Shaw *(Jaume I University)* & Konstantinos Zygalakis *(University of Edinburgh)*

Generative diffusion models are proving to be powerful tools for solving Bayesian inverse problems, delivering highly accurate posterior samples. However, their computational cost is often prohibitive due to the large number of neural evaluations needed per sample—especially in high-dimensional applications like computational imaging, where uncertainty quantification requires many samples. In this talk, I'll present a Multilevel Monte Carlo framework tailored to diffusion-based samplers, which exploits the cost-accuracy trade-offs of these models to drastically cut computational costs. By coupling models of varying precision, we achieve the same final accuracy with up to 4×-to-8× lower computational effort, demonstrated across three benchmark imaging problems.

Equivariant variational auto-encoders for self-supervised Bayesian uncertainty quantification in imaging inverse problems

B. Tamo Amougou, A. Almansa, J. Tachella & **M. Pereyra** *(Heriot-Watt University)*

Imaging problems are often not well posed, leading to significant uncertainty about their solution. Accurately quantifying this uncertainty is critical for the rigorous interpretation of experimental results as well as for reliably using the reconstructed images as quantitative evidence. Unfortunately, existing Bayesian imaging methods are unable to quantify the uncertainty in the reconstructed images in a manner that is robust to experiment replications. This paper presents a new uncertainty quantification methodology based on an equivariant formulation of variational auto-encoders that leverages symmetries and invariance properties commonly encountered in imaging problems. Additionally, the proposed methodology is fully self-supervised and can be trained from observed data alone, thus enabling accurate data-driven uncertainty quantification in situations where there is no ground truth data available. We demonstrate the proposed approach through numerical experiments and comparisons with alternative strategies from the state-of-the-art.

Wavelet-based Physics-Informed Neural Networks

Anshima Singh *(University of Manchester)*, Himanshu Pandey & Ratikanta Behera, *(Indian Institute of Science, Bangalore)*

Physics-informed neural networks (PINNs) face significant challenges when solving differential equations with rapid oscillations, steep gradients, or singular behavior. Considering these challenges, we designed an efficient wavelet-based PINNs (W-PINNs) model to address this class of differential equations. We represent the solution in wavelet space using a family of smooth-compactly supported wavelets. This approach captures the dynamics of complex physical phenomena with significantly fewer degrees of freedom, enabling faster and more accurate training by searching for solutions within the wavelet space. Developed model eliminates the need for automatic differentiation of derivatives in differential equations and requires no prior knowledge about solution behavior, such as the location of abrupt features. In this talk, I will demonstrate how W-PINNs excel at capturing localized nonlinear information through a strategic fusion of wavelets with PINNs, making them particularly effective for problems exhibiting abrupt behavior in specific regions. Our experimental findings show that W-PINNs significantly outperform traditional PINNs, PINNs with wavelets as an activation function, and other state-of-the-art methods, offering a promising approach for tackling challenging differential equations in scientific and engineering applications.

Dissecting Neural Networks

Tiffany Vlaar *(University of Glasgow)*

In this talk I will focus on the role played by individual layers and substructures of deep neural networks. Layer-wise sensitivity to the choice of initialisation and optimiser hyperparameter settings varies. I will show that training neural network layers differ-

ently can lead to enhanced generalisation performance and/or reduced computational cost.

Tensor-to-tensor models with fast iterated sum features

Yue Wu *(University of Strathclyde)* & Joscha Diehl, Rasheed Ibraheem, Leonard Schmitz

We propose a novel tensor-to-tensor layer for deep learning models, particularly focusing on order-2 tensors to provide an image-to-image layer that can be integrated into image processing pipelines. The algorithmic core of our method leverages the mathematical concept of corner trees, originally developed for permutation counting, providing a novel framework for tensor-to-tensor transformations that can effectively handle complex data relationships and structures.

On the one hand, our method can be seen as a higher-order generalization of state space models, which is known to offer promising linear-cost alternatives for sequence-to-sequence tasks. On the other hand, it is based on a multiparameter generalization of the signature of iterated integrals, which has proven successful in summarising stream data over increments while preserving the order of events.

Our experimental results demonstrate the effectiveness of the proposed approach across multiple tasks. In image classification, our method achieves competitive accuracy while reducing the number of trainable parameters by up to 85% and multiply-add operations by up to 65% compared to ResNet architectures. For anomaly detection tasks, our approach achieves remarkable performance, including a 100% AUROC score on the leather category, while maintaining more robust performance with a significantly lower standard deviation (3.9%) compared to conventional approaches (6.3%). These results validate the efficiency and effectiveness of our tensor-to-tensor layer in practical applications.

Convergent algorithms and impossibility results for Koopman operators on reproducing kernel Hilbert spaces

Gustav Conradie *(University of Cambridge)* & Nicolas Boullé, Matthew Colbrook

Data-driven spectral analysis of the Koopman operator is a powerful tool for describing a wide range of real-world dynamical systems, from the behaviour of neurons in mice to variations in sea surface temperatures. The Koopman operator is defined on spaces of functions, and this analysis most commonly takes place on $L^2(\Omega)$. However, defining the Koopman operator on a suitable RKHS has many practical advantages - pointwise predictions and error bounds, more desirable properties of the Koopman operator allowing easier computation, and faster algorithms. In this talk, new algorithms for computing spectra, pseudospectra and spectral measures of Koopman operators on RKHSs will be presented, as well as convergence results and numerical examples. In addition, we discuss impossibility results proving minimum numbers of limits required to compute different parts of the spectrum, showing that our algorithms are optimal in this sense.

Minisymposium M26

The finite element method for problems in multiphysics and geometry - Part 1

Organisers

Francis Aznaran and Shawn Walker

The diffuse interface approach to fluid-structure interaction

Francis R. A. Aznaran & Martina Bukač *(University of Notre Dame, United States)*

We consider the interaction between a (poro)elastic structure and a free-flowing fluid. We propose a diffuse interface model in which a phase field function is used to write each integral in the weak formulation of the coupled problem on the entire domain containing both the fluid and structure regions. The phase field function continuously transitions from one to zero in a diffuse region of width $\mathcal{O}(\epsilon)$ around the interface; this allows the weak forms to be integrated uniformly across the domain, and obviates tracking the subdomains or the interface between them. We prove convergence in weighted norms of a finite element discretisation of the diffuse interface model to the continuous diffuse model. We in turn prove convergence of the continuous diffuse model to the standard, sharp interface, model. Numerical examples verify the proven error estimates, and illustrate application of the method to fluid flow through a complex network, describing blood circulation in the circle of Willis. We also discuss recent work extending this to the large deformation, moving domain case.

High-order finite element methods for multicomponent convection-diffusion

Aaron Baier-Reinio & Patrick E. Farrell *(University of Oxford)*

Multicomponent fluids are mixtures of distinct chemical species (i.e. components) that interact through

complex physical processes such as cross-diffusion and chemical reactions. Additional physical phenomena often must be accounted for when modelling these fluids; examples include momentum transport, thermality and (for charged species) electrical effects. Despite the ubiquity of chemical mixtures in nature and engineering, multicomponent fluids have received very little attention from the finite element community, with many important applications remaining out of reach from numerical methods currently available in the literature. This is in spite of the fact that, in engineering applications, these fluids often reside in complicated spatial regions – a situation where finite elements are extremely useful! In this talk, we present a novel class of high-order finite element methods for simulating cross-diffusion and momentum transport (i.e. convection) in multicomponent fluids. Our model can also incorporate local electroneutrality when the species carry electrical charge, making the numerical methods particularly desirable for simulating liquid electrolytes in electrochemical applications. We discuss challenges that arise when discretising the partial differential equations of multicomponent flow, as well as some salient theoretical properties of our numerical schemes. Finally, we present numerical simulations involving (i) the microfluidic non-ideal mixing of hydrocarbons and (ii) the transient evolution of a lithium-ion battery electrolyte in a Hull cell electrode.

Cause and Cure of Spurious Boundary Forces in an Eulerian Finite Element Method for Moving Domain Flow Problems

Henry von Wahl & Maxim Olshanskii *(Friedrich-Schiller-University Jena)*

We consider the cause and cure of spurious temporal oscillations of boundary forces in the context of an unfitted finite Element for the incompressible Navier–Stokes equations in time-dependent domains. We focus on an Eulerian method for moving domain problems based on cut-FEM. This method enables standard BDF time-stepping by an implicit discrete extension of the solution using ghost-penalty stabilisation to a neighbourhood of the physical domain. We demonstrate that the presence of spurious boundary forces can be explained mathematically by the lack of unconditional stability of the discrete pressure in the $L^\infty(L^2)$-norm. This result is then related to the previous analysis of the moving domain method for the Stokes and linearised Navier-Stokes equations in the literature. We further investigate the dependence of spurious oscillations observed in the Eulerian finite element method on a number of model and discretisation parameters. These results show that the approach is competitive to other approaches to reduce spurious pressure oscillations. Finally, we propose a modification of these methods that is oscillation-free based on the previous analysis.

Anderson acceleration for problems with sparse regularization

Rebecca Durst & Tobin Isaac & Hansol Suh *(Argonne National Laboratory)*

Anderson acceleration/mixing is a common technique applied to fixed-point iterations to accelerate the rate of convergence. The method consists of replacing the traditional update step with a weighted average of previous update steps, with weights chosen to minimize the residuals with respect to previous iterates.

In this developing project, we are interested in applying Anderson acceleration to problems in which a sparsifying regularizer appears in the optimization problem. In the context of multiphysics, these scenarios could arise, for example, in inverse problems involving sparse observations on an interface. In such problems, the resulting optimization problem will typically consist of minimizing the sum of a smooth function and a non-smooth regularizing function, which may be solved using the proximal gradient method. Unfortunately, traditional Anderson acceleration is not considered to be well-suited for use with the proximal gradient method.

Motivated by the potential applications in multiphysics, we develop a novel version of Anderson acceleration for the proximal gradient method on problems with sparse regularization. The method takes advantage of the local linearity of the regularizer functions to equate a proximal gradient update to a gradient descent update in regions where the regularizer is differentiable.

Inf-Sup Stability of Trace Fem for Parabolic Surface PDEs

Lucas Bouck *(Carnegie Mellon University)*

The Trace Finite Element Method (TraceFEM) solves surface PDE problems by using an unfitted mesh in the bulk surrounding a surface and using basis functions in the bulk. This talk considers parabolic problems on a fixed surface. We propose a TraceFEM semidiscrete scheme of the surface heat equation. The key feature of our method is in addition to stabilizing the solution with the normal derivative volume stabilization, we also stabilize the time derivative with a different stabilization scaling. We prove that this scheme satisfies a parabolic inf-sup stability property in the spirit of Tantardini and Veeser (2016). Consequences of inf-sup stability include symmetric error

estimates, optimal rates of convergence under minimal regularity, and additional compactness of discrete solutions, which will be useful for extending to nonlinear problems. This work is joint with R.H. Nochetto (University of Maryland, College Park), M. Shakipov (University of Maryland, College Park), and V. Yushutin (University of Tennessee, Knoxville).

Finite element methods for understanding microswimmer locomotion

Thomas Ranner & Yongxing Wang *(University of Leeds)*

The talk considers an inverse problem for a Cosserat rod where we are given only the position of the midline of the rod and must solve for external forces and torques as well as the orientation of the cross sections of the midline (Wang et al. 2022). The problem is motivated by a dataset of postures of the nematode *Caenorhabditis elegans* moving in 3D space (Ilett et al. 2023). The inverse problem is formulated using an optimal control problem. A monolithic, implicit numerical scheme is proposed using the finite element method. This method combines the mathematical model and laboratory data to study the locomotion of *C. elegans*, which gives us insights into the potential anatomical orientation of the worm beyond what can be observed through the laboratory data. The talk is completed with some ideas of extending the formulation to an embodied 3D model which may allow greater biological insight.

References

Ilett, Thomas P., Omer Yuval, Thomas Ranner, Netta Cohen, and David C. Hogg. 2023. "3D Shape Reconstruction of Semi-Transparent Worms." In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, 12565–75.

Wang, Yongxing, Thomas Ranner, Thomas P. Ilett, Yan Xia, and Netta Cohen. 2022. "A Monolithic Optimal Control Method for Displacement Tracking of Cosserat Rod with Application to Reconstruction of *C. elegans* Locomotion." *Computational Mechanics* 71 (3): 409–32.
https://doi.org/10.1007/s00466-022-02247-x.

Partitioned Methods for Fluid-Poroelastic Structure Interaction Based on Robin Boundary Conditions

Connor Parrow & Martina Bukač *(University of Notre Dame)*

This talk focuses on a novel, strongly-coupled partitioned method for fluid-poroelastic structure interaction and investigates different variations of it. The flow is assumed to be viscous and incompressible, and the poroelastic material is described using the Biot model. To solve this problem, a numerical method based on Robin interface conditions is used, combined with the refactorization of the Cauchy's one-legged 'θ-like' method. In this algorithm, a sequence of Backward Euler–Forward Euler steps is used to discretize the problem in time. In the Backward Euler step, the fluid and poroelastic structure sub-problems are solved iteratively until convergence.Then the Forward Euler step is performed with equivalent linear extrapolations. The finite element method is used for spatial discretization. Variations of further splitting the poroelastic sub-problem into its Darcy and elastic structure sub-problems are also considered. Numerical examples are used to explore convergence and to compare the variations of our method.

Multiscale modelling and simulation of intercellular signalling processes in biological tissues

Mariya Ptashnyk & Chandrasekhar Venkataraman & Sofie Verhees *(Heriot-Watt University & University of Sussex)*

Intercellular signalling processes play crucial role in the interactions and communication between cells in a biological tissue and are involved in all physiological activities of the cells, e.g. division, movement, immune response, tissue development. In the multiscale modelling of intercellular signalling pathways, we consider the dynamics of signalling molecules and cell membrane receptors on the level of a single cell. Using multiscale analysis techniques, we derive macroscopic tissue level description of the intercellular signalling processes. The two-scale bulk-surface finite element method is used for the approximation and numerical simulation of the macroscopic models. To analyse the interplay between the signalling pathways and mechanics, we consider a two-way coupling between the chemical processes and elastic deformations of cells.

Implicit-explicit schemes for incompressible flow problems with variable viscosity and density

Gabriel R. Barrenechea *(University of Strathclyde)*

This talk is devoted to the of study different Implicit-Explicit (IMEX) schemes for incompressible flow problems with variable viscosity, and density. Unlike most previous work on IMEX schemes, which focuses on the convective part, we here focus on treating parts of the diffusive term explicitly to reduce the coupling

between the velocity components. In the first part of the talk we present the main idea and different, both monolithic and fractional-step, IMEX alternatives for the variable-viscosity Navier–Stokes system, analysing their theoretical and algorithmic properties, and their numerical performance [1]. Then, we move onto the Navier-Stokes equation with variable density, where we apply these ideas to generate unconditionally stable, linearised IMEX schemes, both monolithic and fractional-step. Our presentation is restricted to the semi-discrete case, only considering the time discretisation. In this way, the results herein can be applied to any spatial discretisation. We finally present tests based on a finite element discretisation in space, ranging from simple manufactured solutions to complex two-phase viscoplastic flows [2].

The results presented in this talk were obtained in collaboration with Ernesto Castillo (USACH, Chile), and Nicolás Espinoza-Contreras and Douglas R. Q. Pacheco (RWTH Aachen University, Germany).

References

[1] Barrenechea, G.R., Castillo, E., and Pacheco, D.R.Q. "Implicit-explicit schemes for incompressible flow problems with variable viscosity." SIAM J. Sci. Comput. **46**(4), A2660–A2682, (2024).

[2] Espinoza-Contreras, N., Barrenechea, G.R., Castillo, E., and Pacheco, D.R.Q. "Unconditionally stable, linearised IMEX schemes for incompressible flows with variable density." arXiv preprint arXiv:2410.11510.

Minisymposium M27

The finite element method for problems in multiphysics and geometry - Part 2

Organisers
Francis Aznaran and Shawn Walker

Sensitivity analysis of minimization diagrams and applications

Antoine Laurain *(University of Duisburg-Essen)*

Minimization diagrams encompass a large class of diagrams of interest in the literature, such as generalized Voronoi diagrams. We develop an abstract perturbation theory in two dimensions and perform a sensitivity analysis for functions depending on sets defined through intersections of smooth sublevel sets, and formulate precise conditions to avoid singular situations. This allows us to define a general framework for solving optimization problems depending on two-dimensional minimization diagrams. The particular case of Voronoi diagrams is discussed to illustrate the general theory. A variety of numerical experiments is presented, which show that the proposed methodology allows the construction of customized Voronoi diagrams using off-the-shelf well-established optimization algorithms.

Finsler geodesics and finite-strain plasticity

Oliver Sander *(TU Dresden)*

The theory of energetic rate-independent systems is an elegant way to describe nonlinear systems in mechanics and other fields. One particular advantage is that it yields a natural time discretization that consists of a sequence of minimization problems. Unfortunately, in many interesting cases the objective functional is only given implicitly as the solution of a second minimization problem for a curve length in the state space. Therefore, its evaluation and obtaining derivatives can be very costly. Instead, we present a transformation based on the Finsler exponential map that turns the second minimization problem into an initial-value-problem for a second-order ODE. Solutions of this can be found much cheaper numerically, or may even be available in closed form. We show examples of this construction, and how to use it to obtain fast and robust Proximal Newton solvers for finite-strain elastoplasticity.

Exploring physics-dynamics coupling with compatible finite element discretisations of moist shallow water equations

Nell Hartney, Jemma Shipton *(University of Exeter)* & Thomas Bendall *(Met Office)*

At the heart of any weather or climate model is the dynamical core, which computes solutions to the atmospheric fluid equations (known as the dynamics). Processes not captured by the dynamical core which nonetheless have an important impact on the overall flow are known as the physics. These processes are parametrised separately and coupled to the dynamical core to allow them to influence the solution correctly. The implementation of this so-called physics-dynamics coupling can have a significant impact on the effectiveness of a model and there are many challenges associated with it, including how physics should be dealt with in the model's timestep.

The moist shallow water equations offer a useful context to explore some of these physics-dynamics coupling questions. Including moisture in the traditional shallow water equations introduces physics into what is otherwise a dynamics-only model, giving an inex-

pensive framework that couples a physics process to simple (but reasonably realistic) dynamics.

This talk will describe our implementation of a number of different moist shallow water models using the compatible finite element method. Our model is constructed using Gusto, the dynamical core toolkit that builds on the Firedrake finite element library. I will describe how we have discretised the moist shallow water equations using compatible finite elements in Gusto, and how we have used moist shallow water test cases to explore some of the implications of different modelling choices, as well as investigating questions about physics-dynamics coupling and how physics is dealt with by a model's time-stepping scheme.

HSS iteration for solving the indefinite Helmholtz equation by multigrid with standard components

Colin Cotter & Joshua Hope-Collins *(Imperial College London)* & Kars Knook *(University of Oxford)*

We present, analyse and demonstrate an iterative solution approach for the finite element discretisation of the indefinite Helmholtz problem. The approach is based on Hermitian Skew-Hermitian Splitting (HSS) iterations, in combination with shift preconditioning (using a preconditioner with k^2 replaced by $k^2 + i\epsilon$ for shift $\epsilon > 0$. Gander, Graham and Spence (2015) showed that the shift must be $\mathcal{O}(k)$ in order for preconditioned GMRES to converge in $\mathcal{O}(1)$ iterations as $k \to \infty$. This is important because GMRES has a cost proportional the square of the iteration count. On the other hand, Cocquet and Gander (2017) showed that the shift must be $\mathcal{O}(k^2)$ if the preconditioning operator is to be robustly approximated using a multigrid method with standard smoothers (e.g. scaled Jacobi) and transfer operators. To bridge this gap, we introduce a preconditioner consisting of HSS iterations with suboptimal parameter leading to a shifted problem with $\mathcal{O}(k^2)$ shift. We prove that if one preconditioner application consists of $\mathcal{O}(k)$ HSS iterations, then preconditioned GMRES converges in $\mathcal{O}(1)$ iterations. We then demonstrate this result using numerical experiments, and show further that the method produces a solution in $\mathcal{O}(k)$ wallclock time given sufficiently many computational cores, when multigrid is used to approximate the solves in the HSS iterations.

Isoparametric finite element methods for mean curvature flow and surface diffusion

Ganghui Zhang *(University of Edinburgh)*, Harald Garcke *(Universität Regensburg)*, Robert Nürnberg *(Università di Trento)* & Simon Praetorius *(Technische Universität Dresden)*

We propose higher-order isoparametric finite element approximations for mean curvature flow and surface diffusion. The methods are natural extensions of the piecewise linear finite element methods introduced by Barrett, Garcke, and Nürnberg (BGN) in a series of papers in 2007 and 2008. The proposed schemes exhibit unconditional energy stability and inherit the favorable mesh quality of the original BGN methods. Moreover, in the case of surface diffusion we present structure-preserving higher-order isoparametric finite element methods. In addition to being unconditionally stable, these also conserve the enclosed volume. Extensive numerical results demonstrate the higher-order spatial accuracy, the unconditional energy stability, the volume preservation for surface diffusion, and the good mesh quality.

Minisymposium M28

Advances in numerical analysis techniques for complex networks

Organisers
Francesca Arrigo and Dario Fasino

A new walk-based centrality index for directed acyclic networks

Daniele Bertaccini & Luigi Chiricosta & **Alessandro Filippo** *(University of Rome Tor Vergata)*

Many real-world cascade processes can be described as source-to-sink paths in a directed acyclic graph (DAG), where the source node represents the triggering event and the sink node represents the final outcome. Therefore, in such acyclic networks, it makes sense to count the number of source-to-sink paths in which a node participates to measure its importance (or centrality) in the network. In fact, the higher the number of those paths that visit a node, the higher the number of cascade reactions that will be affected by the removal/failure of that specific node.

In this talk, based on a joint work with D. Bertaccini and L. Chiricosta, we present a novel walk-based centrality measure to rank nodes in a DAG along with an efficient way of computing and updating it after the removal of an edge. We also discuss a possible application to the analysis of biological pathways.

References

[1] M. Benzi and C. Klymko, Total communicability

as a centrality measure, *Journal of Complex Networks*, **1**(2), pp. 124–149, 2013.

[2] D. Bertaccini, L. Chiricosta, and A. Filippo, Source-to-sink communicability: a new centrality measure for directed acyclic networks, *submitted*.

[3] E. Estrada and D. J. Higham, Network properties revealed through matrix functions, *SIAM Review*, **52**(4), pp. 696–714, 2010.

[4] P. Naderi Yeganeh, C. Richardson, E. Saule, A. Loraine, and M. T. Mostafavi, Revisiting the use of graph centrality models in biological pathway analysis, *BioData Mining*, **13**, 2020.

Role extraction in directed networks by generalised random walks

Dario Fasino *(University of Udine)*

The nodes in a network can be grouped into equivalence classes according to their connection patterns with other nodes, whether in the same group or different ones. This process, known as role extraction or block modelling, typically involves defining a pairwise node similarity matrix and then clustering the rows and columns of this matrix. Additionally, the similarity matrix can be replaced by a low-rank approximation to reduce memory and computational costs. Arnaud Browet and Paul Van Dooren defined a node similarity matrix to solve the role extraction problem in directed networks as the solution to a suitable matrix equation, solved iteratively. Here, I propose a variant of the Browet–Van Dooren method that introduces appropriate diagonal scalings of the adjacency matrix to compensate for the inhomogeneity of node connections. The underlying idea is to figure out node roles using random walks that move in both the forward and backward directions along the links. Compared to the Browet–Van Dooren method, theoretical properties and numerical experiments demonstrate superior performance, particularly in networks with heterogeneous node degree distributions.

This work was supported by the Italian Ministry of University and Research through the PRIN Project 20227PCCKZ "Low Rank Structures and Numerical Methods in Matrix and Tensor Computations and their Applications". The author is also affiliated to the INdAM-GNCS.

Modeling advection on distance-weighted directed networks

Francesco Zigliotto & Michele Benzi & Fabio Durastante *(Scuola Normale Superiore)*

In this talk, we introduce a mathematical model to capture and describe the dynamics of the advection differential equation on distance-weighted directed graphs, with applications to various networked systems. The primary objective of our model is to generalize advection processes — which traditionally describe phenomena like fluid flow or traffic movement — by formulating them within the framework of discrete network structures.

Our approach begins with defining a set of essential properties, or axioms, that any discrete advection operator must satisfy. These axioms ensure that the operator reflects the fundamental characteristics of advection processes in continuous spaces, such as directional flow, conservation properties, and respect for edge weights based on distance. We demonstrate that, under these conditions, there exists an essentially unique operator that fulfills all prescribed axioms, providing a robust and mathematically sound foundation for discrete advection on directed graphs.

To validate our theoretical results, we present both analytical and numerical examples that showcase the operator's behavior under various configurations. As a practical demonstration, we apply the model to simulate traffic flow in a transportation network.

Interlacing of centrality measures and cospectral vertices

Nikita Deniskin *(Scuola Normale Superiore)*

Centrality measures are used to find the most important nodes in a network. What "important" means is highly dependent on the setting. Therefore, there are many possible measures, which give birth to different rankings of the vertices. We focus on walk-based centrality measures, which depend on a real parameter. Changing the value of the parameter can result in a swap in the ranking for two vertices, called *interlacing*. Just like comparing different rankings, studying interlacing gives us insight on the role of the vertices and on the characteristics of the chosen centrality measures.

It is possible that two vertices will always have the same score for a family of centrality measures, despite not being indistinguishable in the graph (i.e, related by an automorphism). They are called *cospectral vertices*, and they provide a connection to spectral graph theory.

Quantum walks are the equivalent of random walks on a graph. If two vertices are *strongly cospectral*, then perfect state transfer can occur in the random walk. This is an important and non-trivial problem

in a quantum computing setting because it is difficult to transfer a quantum state: it cannot simply be copied, and attempts at recreating it through measuring would destroy it.

In this talk, we study interlacing and properties of cospectral vertices in the context of centrality measures, with the aim of presenting open questions and giving insight on the connections between the different fields of study (Network Science, Spectral Graph Theory, Quantum Computing).

Katz Centrality for Signed Networks

Shuruq Alharbi *(University of Strathclyde)*

Centrality is a widely used concept to figure out how a node is important in a network. In contrast to unsigned networks, little attention has been paid to the use of centrality in signed networks that include both positive (e.g., friendship, alliance) and negative (e.g., rivalry, competition) relations. In this talk, we present variants of Katz centrality suitable for signed networks. We discuss why studying centrality is crucial and how the negative relations can change centrality scores. We also address the problem of picking a parameter value for Katz centrality that ensures that our measure is positive for all nodes with some new theoretical results along with some numerical experiments.

Abstracts of Contributed Talks

Rational methods for abstract, initial boundary value problems without order reduction

Carlos Arranz-Simón & Begoña Cano & César Palencia *(University of Valladolid)*

It is well known that a Runge-Kutta method of order p suffers from the so called order reduction phenomenon when it is applied to time integrate a parabolic or hyperbolic PDE. In this work, we part from the rational mappings of some RK methods to propose a family of stable numerical schemes of order p, thus avoiding order reduction.

To this end, we consider the numerical time integration of abstract, initial boundary value problems of the form

$$\begin{cases} u'(t) = Au(t) + f(t, u(t)), \quad t > t_0, \\ u(0) = u_0, \\ \partial u(t) = g(t), \quad t > t_0, \end{cases}$$

where $A : D(A) \subset X \to X$ is the infinitesimal operator of a $\mathcal{C}_0$ semigroup of linear, bounded operators in a Banach space X, $\partial : D(A) \subset X \to X$ is a linear operator and $u_0 \in X$, $f : [t_0, \infty) \times X_\alpha \to$ and $g : [t_0, \infty) \to X_b$. This abstract framework covers a wide variety of situations of practical interest, including both parabolic problems (reaction-diffusion, Schrödinger, etc) and hyperbolic problems (wave equations, Navier-Stokes, etc).

The numerical methods that we present achieve order of convergence p using only evaluations of the source term f and not of its derivatives. They can be implemented in an efficient way that, after some initial steps, requires the following computational cost per step:

- an evaluation of the source term f,
- solving an elliptic problem associated with $g(t)$,
- solving s linear systems, as in the original RK methods.

Finally, we explain how predictor-corrector like schemes can be implemented to improve the error and the stability of these methods.

A relaxation Crank-Nicolson scheme for the von Neumann equation with power nonlinearity

Agissilaos Athanassoulis & Fotini Karakatsani *(University of Dundee)*

We propose a novel numerical method for the von Neumann equation with power nonlinearity and homogeneous background. This equation, also known as Alber equation, appears in the study of stochastic ocean waves [1] and reads

$$\begin{aligned} i\partial_t u + p(\Delta_x - \Delta_y)u + q\Big(V(x,t) - V(y,t)\Big) \\ \Big(\Gamma(x-y) + u(x,y,t)\Big) = 0, \qquad (1) \\ V(x,t) = u(x,x,t), \qquad u(x,y,0) = u_0(x,y), \end{aligned}$$

where p and q are real-valued parameters, and u_0 is Hermitian, $u_0(x,y) = \overline{u_0(y,x)}$.

Γ is the autocorrelation of the homogeneous background sea state, and u is a localized inhomogeneity. The main phenomenon is a bifurcation between a stable regime (Landau damping, where the inhomogeneity disperses) and an unstable regime (modulation instability, where the inhomogeneity feeds of the homogeneous background and grows) [1, 3, 4, 5, 2].

There are only two papers dealing with the numerical solution of the Alber equation, [6] and [5]. These works are fundamental for this problem, and they highlight the challenges this non-standard equation poses. Both papers use a forward Euler method for time-stepping, and finite differences in space.

We introduce a relaxation Crank-Nicolson scheme, which preserves at the discrete level the L^2 balance law of equation (1). Fourth-order finite differences are used in space, and subtle issues related with the initialization of the scheme are investigated. Numerical results include exact solutions, and both stable and unstable sea states.

Finally, the relationship with the broader class of von Neumann and Wigner equations is discussed, along with the state of the art and challenges in their numerical solution.

References

[1] Alber, I. The effects of randomness on the stability of two-dimensional surface wavetrains. *Proc. R. Soc. Lond. A*, **363** (1978), 525–546.

[2] Athanassoulis, A., Athanassoulis, G., Ptashnyk, M. & Sapsis, T. Strong solutions for the Alber equation

and stability of unidirectional wave spectra. *Kinetic and Related Models*, **13** (2020), 703–737.

[3] Athanassoulis, A. G., Athanassoulis, G. A. & Sapsis, T. Localized instabilities of the Wigner equation as a model for the emergence of rogue waves. *Journal of Ocean Engineering and Marine Energy*, **3** (2017), 325–338.

[4] Onorato, M., Osborne, A., Fedele, R. & Serio, M. Landau damping and coherent structures in narrow-banded deep-water gravity waves. *Physical Review E*, **67** (2003), 046305.

[5] Ribal, A., Babanin, A. V., Young, I., Toffoli, A. & Stiassnie, M. Recurrent solutions of the Alber equation initialized by Joint North Sea Wave Project spectra. *Journal of Fluid Mechanics*, **719** (2013), 314-344.

[6] Stiassnie, M., Regev, A. & Agnon, Y. Recurrent solutions of Alber's equation for random water-wave fields. *Journal of Fluid Mechanics*, **598** (2008), 245–266.

Alternating Direction Method of Multipliers (ADMM) for Nonlinear Matrix Decompositions

Atharva Awari (*University of Mons)*

Low-rank matrix approximations are fundamental in data analysis, machine learning, and signal processing. Traditional approaches, such as singular value decomposition (SVD) and non-negative matrix factorization (NMF), assume a linear relationship between the observed data matrix X and its low-rank factors W and H. However, many real-world datasets exhibit nonlinear structures that cannot be effectively captured using standard linear models. This has led to growing interest in nonlinear matrix decompositions (NMDs), where the goal is to find low-rank factors W and H such that $X \approx f(WH)$, where f is a nonlinear function applied element-wise. Despite the increasing relevance of NMDs, existing algorithms lack the flexibility to handle a wide range of nonlinear functions commonly used in practice. Examples include the ReLU function with $f(x) = \max(0, x)$) useful in the approximation of sparse datasets, the component-wise square with $f(x) = x^2$ useful in the representation of probabilistic circuits, and Min-Max models where the data lie in a certain interval (a,b) with $f(x) = min(b, max(a, x))$. Current methods also do not support other loss functions than least squares, which is essential in some applications. To bridge this gap, we propose an Alternating Direction Method of Multipliers (ADMM) framework tailored for NMDs. Our method efficiently handles diverse nonlinear models while accommodating different loss functions, including least squares, the l1 norm, and the Kullback-Leibler divergence. Furthermore, our approach is easily adaptable to other nonlinear functions and loss functions, ensuring broad applicability in future research.

A Nitsche Approach for Coupled Multiphysics Problems

Aparna Bansal & Nicolás A. Barnafi, Ricardo Ruiz-Baier, Dwijendra Narain Pandey *(Indian Institute of Technology Roorkee)*

In this work, we present a model for the interaction between free fluid flow and a poroelastic medium. The Brinkmann is employed to describe the fluid flow within the porous structure, accounting for inertial effects. A thermodynamically consistent formulation is established for soft tissue perfusion. To approximate the solution numerically, we develop a mixed finite element method based on Nitsche's approach and prove the well-posedness of the discrete formulation. Additionally, we derive *a priori* error estimates in the energy norm. Numerical experiments are performed to validate the theoretical convergence rates and demonstrate the method's effectiveness in capturing the relevant physical phenomena.

A posteriori error control for a finite volume scheme for a cross-diffusion model of ion transport

Arne Berrens & Jan Giesselmann *(TU Darmstadt)*

We consider the ion transport model

$$\partial_t u_i = \nabla \cdot (u_0 \nabla u_i - u_i \nabla u_0) \quad \forall i = 1, \dots, n, \text{ on } \Omega \times [0, T]$$

where Ω is a bounded Lipschitz domain, $T > 0$ and $u_1, \dots,$
u_n describe the ion concentrations and u_0 is the concentration of the solvent. Here we impose mixed Dirichlet-Neumann boundary conditions and volume-filling i.e. $\sum_{i=0}^{n} u_i = 1$. The system models the transport of ions through relatively small geometries where the size of individual molecules is not negligible. Hence, the diffusion of each ion species is influenced by the diffusion of all the other species, due to the size exclusion effects.

We use a standard technique to numerically solve the above system, more precisely a cell-centered finite volume method in space and implicit Euler in time. To obtain the residual based a posteriori error bound, we

use an abstract L^2 stability framework and a reconstruction of the piecewise constant finite volume solution to get a continuous piecewise polynomial approximate solution. A key step in the derivation is to develop an a posteriori L^∞ in space and time error bound for the solvent concentration u_0, which solves a diffusion equation. We think, this result is interesting in its own right. Numerical experiments indicate that the a posteriori error estimator has the same rate of convergence as the actual error.

Randomized algorithms with random Khatri-Rao product matrices

Zvonimir Bujanović *(University of Zagreb)*

Randomized algorithms have gained significant attention in numerical linear algebra during the last decade. In particular, randomized sketching is used as a simple but effective technique in which a random matrix acts as a dimension reduction map: a problem that features a potentially large input matrix $A \in \mathbf{R}^{n\times n}$ is reduced to a smaller one by replacing A with $A\Omega$, where $\Omega \in \mathbf{R}^{n\times \ell}$ is a random matrix with $\ell \ll n$. This has been used with great success in, e.g., randomized SVD and subspace projection methods for large-scale eigenvalue problems, such as FEAST.

Algorithms based on sketching typically draw random matrices Ω from standard distributions, such as Gaussian. However, in certain applications it may be advantageous to run computations with Ω that is compatible with the underlying structure of the problem. In this talk we discuss algorithms that use random Khatri-Rao product matrices: each column of Ω is generated as the Kronecker product of two Gaussian random vectors. This will allow for faster operations when the matrix A is represented as a short sum of Kronecker products, which arises frequently, e.g., from the discretization of PDEs on tensor product domains. We focus on applications in large-scale eigenvalue computation, and provide theoretical and numerical evidence that the use of random Khatri-Rao product matrices Ω instead of unstructured Gaussian random matrices leads to good estimates.

This is joint work with Luka Grubišić, Daniel Kressner, and Hei Yin Lam.

Residual a posteriori error estimates with boundary correction for φ-FEM

Raphaël Bulle *(Inria de l'Université de Lorraine)* & Roland Becker *(University of Pau)* & Michel Duprez *(Inria de l'Université de Lorraine)* & Vanessa Lleras *(University of Montpelllier)*

φ-FEM is an immersed boundary finite element method that does not require any unconventional numerical integration on cut elements or on the boundary. This difficulty is avoided by the introduction of a level-set function in the discrete formulation. In this talk, we introduce an a posteriori error estimator for the φ-FEM discretization of Poisson-Dirichlet boundary values problems. This novel residual type estimator has the particularity to control the boundary approximation error via a dedicated term, making it particularly well suited to steer adaptive refinement loops for problems defined on domains with complicated shapes. We give the key ingredients of the proof of the estimator reliability and show how we can take advantage of the capabilities of the FEniCSx software to easily implement an adaptive refinement loop based on this estimator. Finally, we illustrate the performances of this estimator on several numerical examples.

Error estimates for full discretization by an almost mass conservation technique for a Cahn–Hilliard system with dynamic boundary conditions

Nils Bullerjahn *(Paderborn University)*

In this talk we present a novel technique for achieving optimal-order error estimates for the full discretization by linear bulk–surface finite elements in space and by the linearly implicit backward difference method of order 1 to 5 in time. The new idea for the stability analysis uses mass conservation properties of the equation to conclude an *almost mass conservation* of the error, and combines this with a Poincaré-type estimate and an energy estimate. The fully discrete consistency bounds are obtained, by error estimates for the spatial discretization and a sufficiently regular extension of the extrapolation by a Hermite interpolation to obtain error estimates for the backward difference time discretization. This provides optimal-order error estimates between the solution of the numerical scheme and a sufficiently regular exact solution.

We apply this technique to the recently developed bulk–surface Cahn–Hilliard system with general dynamic boundary conditions, which includes a number of important previously known dynamic boundary conditions of Cahn–Hilliard-type, such as the Goldstein–Miranville–Schimperna-model, the Liu–Wu-model and the reaction rate dependent dynamic boundary conditions.

We expect that these techniques can be transferred to other similar equations, satisfying an energy estimate and mass conservation properties, other important examples include Allen–Cahn and Cahn–Hilliard equa-

tions in stationary domains with classical boundary conditions, or the same partial differential equations on evolving surfaces.

Numerical experiments are presented to illustrate and complement the theoretical results.

A Quantum Super-Krylov Diagonalization Method

Adam Byrne & William Kirby & Kirk M. Soodhalter & Sergiy Zhuk *(Trinity College Dublin, IBM Research)*

The problem of estimating the ground-state energy of a quantum many-body system is ubiquitous in chemistry and condensed matter physics. For a system of n qubits, this problem reduces to computing the minimum eigenvalue of an order-2^n Hermitian matrix H, which is an exponentially hard task on classical computers due to the cost of storing vectors in the 2^n-dimensional Hilbert space. Krylov quantum diagonalization (KQD) algorithms have emerged as a potential approach to overcome this storage problem by encoding the Hilbert space of the system in the exponentially-sized Hilbert space of a register of quantum bits. The time evolution $U(t) = e^{-\imath Ht}$ can be efficiently approximated by a quantum device via discretisation techniques, so the most natural choice of projection space is that spanned by the vectors $|v_k\rangle = U^k(t)|v\rangle$, for some initial state $|v\rangle$ and $t > 0$. It can be shown that the error in the resulting ground-state energy estimate converges exponentially quickly with the Krylov dimension. However, in practise, unless H has some additional structure, these algorithms rely on subroutines which are prohibitively difficult for near-term quantum computers. Motivated by this, we propose a KQD method that can be efficiently performed by existing quantum computers, and exhibits convergence behaviour similar to that of standard KQD methods. This method employs the Rayleigh-Ritz procedure to approximate the eigenvalues of the super-operator

$$\mathcal{J}_H : \mathcal{M}_{2^n}(\mathbb{C}) \to \mathcal{M}_{2^n}(\mathbb{C}), \quad \mathcal{J}_H(X) := \imath(HX - XH), \tag{1}$$

where $\mathcal{M}_{2^n}(\mathbb{C})$ is the Hilbert space of order-2^n complex matrices equipped with the trace inner product. Denote the eigenvalues of H by $\lambda_1 \leq ... \leq \lambda_{2^n}$, so the eigenvalue of $\mathcal{J}_H$ with smallest imaginary part is $\delta_1 := \imath(\lambda_1 - \lambda_{2^n})$. Then given an estimate of δ_1, one can estimate the ground-state energy λ_1 of H in the following cases: (1) if H has symmetric spectrum $\lambda_{2^n} = -\lambda_1$ so $\lambda_1 = \delta_1/2\imath$, or (2), if λ_{2^n} is known so $\lambda_1 = \delta_1/\imath + \lambda_{2^n}$. We provide a wide range of example Hamiltonians satisfying these conditions. Similar to standard KQD methods, we use the projection space

$$\begin{aligned}\mathcal{K} &:= \operatorname{span}\left\{\rho_0, ..., \rho_{m-1}\right\} \\ &= \left\{ \sum_{j=0}^{m-1} \alpha_j \rho_j \ \in \mathcal{M}_{2^n}(\mathbb{C}) : \ \alpha_j \in \mathbb{C} \right\}\end{aligned} \tag{2}$$

where $\rho_j := |v_j\rangle\langle v_j| \in \mathcal{M}_{2^n}(\mathbb{C})$ and $m > 0$ is some integer parameter. We seek an approximate eigenpair $(\widetilde{\delta}, \widetilde{\Delta}) \in \imath\,\mathbb{R} \times \mathcal{K}$ satisfying the Galerkin condition $\left(\mathcal{J}_H(\widetilde{\Delta}) - \widetilde{\delta}\widetilde{\Delta}\right) \perp \mathcal{K}$. This yields an $m \times m$ projected eigenvalue problem

$$A\mathbf{x} = \widetilde{\delta} B\,\mathbf{x}. \tag{3}$$

It turns out that the entries of the projected matrices in (3) can be written as

$$\begin{aligned} A_{jk}(t) &= \frac{1}{(j-k)}\frac{d}{dt}B_{jk}(t), \\ B_{jk}(t) &= |\langle v|U^{-j}(t)U^k(t)|v\rangle|^2. \end{aligned} \tag{4}$$

The real-time evolutions $|v\rangle \mapsto U^k(t)|v\rangle$ are approximated on a quantum device and the matrix B is constructed entry-wise by performing the overlaps in (4) on a device. These operations can both be efficiently performed by existing quantum computers. For the matrix A, we propose a *classical* derivative estimation algorithm for approximating $\frac{d}{dt}B_{jk}(t)$, given some noisy *quantum* measurements of $B_{jk}(t)$. Then A is classically constructed entry-wise using the relation in (4). Finally, the problem (3) is solved classically and the minimum eigenvalue $\widetilde{\delta}_1$ serves as an estimate of δ_1. We prove that the error $|\delta_1 - \widetilde{\delta}_1|$ converges exponentially quickly with respect to m, and provide classical numerical simulations for various large-scale ($n \geq 100$) Hamiltonians.

A finite element method for a perturbed Navier-Stokes Problem arising from 4D-Flow MRI.

Cristian Cárcamo & Gabriel Barrenechea & Abner Poza *(Weierstrass Institute)*

This work introduces a mathematical model grounded in the Navier–Stokes equations, aimed at reconstructing pressure fields from known velocity data. We formulate the problem within a continuous framework and identify sufficient conditions under which the model is well-posed. A preliminary scheme is proposed for the estimation of arterial pressure based on 4D-Flow MRI measurements. The numerical method employed is detailed, and a set of theoretical results is established in order to prove the existence and uniqueness of solutions, along with the specific conditions that guarantee well-posedness. An error analysis is carried out by applying standard finite element techniques, and numerical experiments are presented to

validate the theoretical results. These simulations further confirm the robustness of the method when applied to non-analytic, experimentally-derived data, illustrating its possible and potential applicability in biomedical contexts.

Efficient solution of Cahn-Hilliard-Navier-Stokes models for organic solar cell production

Pelin Çiloğlu & Carmen Tretmans & Roland Herzog & Jan-F. Pietschmann & Martin Stoll *(TU Chemnitz)*

In this talk, we investigate the numerical behavior of coupled Cahn–Hilliard-Navier–Stokes models for morphology formation within the active layer of organic solar cells. The model describes the dynamics of a polymer, a non-fullerene acceptor, and a solvent through Cahn–Hilliard equations, coupled with the Navier–Stokes equations to capture macroscopic fluid motion. To account for solvent evaporation, we incorporate an Allen–Cahn equation into the framework. The system is discretized using a finite element method in space and a semi-implicit time-stepping scheme.

The resulting (non)linear systems are large-scale and tightly coupled, leading to significant computational challenges. We propose a preconditioned iterative scheme that solves these coupled equations efficiently and remains robust with respect to discretization parameters. Numerical experiments demonstrate the effectiveness of the model and the proposed methodology through several examples.

A biologically-driven FEM framework for mixed-dimensional PDEs on evolving realistic geometries

Alessandro Contri & André Massing & Padmini Rangamani *(NTNU - Norwegian University of Science and Technology) - (UCSD - University of California San Diego)*

We present a finite element framework targeted at simulating biologically inspired phenomena involving moving boundaries such as chemotaxis and structural plasticity. The continuum-mechanics based modeling of such membrane processes often lead to complex systems of partial differential equations (PDEs) with numerous computational challenges, including mixed-dimensional coupling of surface and bulk PDEs, and free interface/boundary problems where the domain evolution itself it governed by the system to be solved. In this talk, we demonstrate how this challenges can be addressed by combining and extending state-of-art discretization methods for evolving domain and surface problems.

The first challenge we address is constituted by the reacting species, often described by a system of nonlinearly coupled diffusion-advection-reaction equations. Although the Surface FEM (SFEM) theory for parabolic PDEs on moving domains is well-established, less is known about advection-dominant problems. We propose a stabilized SFEM for open surfaces employing the continuous interior penalty (CIP) method [1] to deal with the vanishing viscosity cases. This is complemented with the mass- and bound-preserving postprocessing of [3] to maintain the species in the physically relevant range. Another challenge is the simulation of the elastic behavior of the cellular membrane, which often moves under gradient flow. We enhance cutting-edge algorithms in the field to be able to deal with realistic mesh geometries resulting from modern cell imaging technology. The stable algorithm [5] for boundary value problems for Willmore flow is augmented with the mean-curvature stabilization proposed in [1]. A subsequent post-processing stage applies the mesh-redistribution algorithm [2] to maintain mesh quality.

Convergence studies on idealized geometries are presented to prove the accuracy of the proposed algorithms. Extensive simulations on real geometries are also presented to prove the reliability of the presented simulation pipeline.

References

[1] P. Hansbo, M. G. Larson, and S. Zahedi. Stabilized finite element approximation of the mean curvature vector on closed surfaces. *SIAM Journal on Numerical Analysis*, 2015.

[2] B. Duan and B. Li. New artificial tangential motions for parametric finite element approximation of surface evolution. *SIAM Journal on Scientific Computing*, 2024.

[3] Q. Cheng and J. Shen. A new Lagrange multiplier approach for constructing structure preserving schemes, II. Bound preserving. *SIAM Journal on Numerical Analysis*, 2022.

[4] E. Burman. A unified analysis for conforming and nonconforming stabilized finite element methods using interior penalty. *SIAM Journal on Numerical Analysis*, 2005.

[5] J. W. Barrett, H. Garcke, and R. Nürnberg, Stable variational approximations of boundary value problems for Willmore flow with Gaussian curvature. *IMA*

Journal of Numerical Analysis, 2017.

Numerical approximation of the Munk equation with a compact scheme

Jean-Pierre Croisille & Matania Ben-Artzi & Dalia Fishelov *(Université de Lorraine)*

The 2D linear Munk equation is the convection-diffusion equation $-\beta.\nabla u + \varepsilon\Delta^2 u = f$ where $\beta \in \mathbf{R}^2$ and $\varepsilon > 0$ are parameters. This is a model for the closed ocean circulation with sharp western boundary layers, which obeys the nonlinear barotropic equation. In this study we show that high order compact schemes previously introduced in other contexts are applicable and yield good results. The difficulty involves the accuracy of the scheme when the parameters lead to singularities, namely, $|\beta| \to +\infty$, $\varepsilon \to 0$. In this case, it is impossible to use a uniform grid on the whole domain. On the contrary, we show that it is possible to define a multiscale version of the scheme at transmission nodes, preserving the high order accuracy. Numerical results are presented, based on test cases in [2]. The 1D equation $-\beta\dfrac{d}{dx}u + \varepsilon\dfrac{d^4}{dx^4}u = f$ is considered for the design of the scheme as well as for convergence proofs, using discrete functional analysis or alternatively matrix algebra tools.

References

[1] M. Ben-Artzi, J.-P. Croisille and D. Fishelov. Navier-Stokes equations in planar domains. Imperial College Press, (2013).

[2] M.D. Chekroun, Y. Hong and R.M. Temam. Enriched numerical scheme for singularly perturbed baro-

tropic Quasi-Geostrophic equations. J. Comput. Phys., 416, (2020).

[3] P.A. Farrell, A.E. Hegarty, J.J.H. Miller, E. O´Riordan and G.I. Shishkin. Robust computational techniques for boundary layers. Chapman and Hall CRC, (2000).

Spectral Properties of Infinitely Smooth Kernel Matrices in the Single Cluster Limit, with Applications to Multivariate Super-Resolution

Nuha Diab & Dmitry Batenkov *(Tel-Aviv University)*

We study the spectral properties of infinitely smooth multivariate kernel matrices when the nodes form a single cluster. We show that the geometry of the nodes plays an important role in the scaling of the eigenvalues of these kernel matrices. For the multivariate Dirichlet kernel matrix, we establish a criterion for the sampling set ensuring precise scaling of eigenvalues. Additionally, we identify specific sampling sets that satisfy this criterion. Finally, we discuss the implications of these results for the problem of super-resolution, i.e. stable recovery of sparse measures from bandlimited Fourier measurements.
https://arxiv.org/abs/2407.10600.

Adaptive RBF cubature method for scattered data on spherical polygons

Giacomo Elefante & Roberto Cavoretto, Alessandra De Rossi, Alvise Sommariva *(USI Lugano)*

We implement an adaptive method for numerical cubature from scattered data over spherical polygons based on Radial-Basis Functions (RBF), in particular Radial-Powers (RP) or Thin-Plate Splines (TPS) interpolation with near-optimal data-driven exponent.

Key ingredients for this algorithm are, firstly, a choice of the shape parameter guided by a variant of LOOCV method suited for cubature and, secondly, a novel adaptive routine for computing integrals over these kind of domains.

Pointwise error bounds in POD methods without difference quotients

Bosco García-Archilla & Julia Novo *(Universidad de Sevilla)*

There is an ongoing debate on wether it is necessary to include the difference quotients (DQs) of the snapshots in the dataset in proper orthogonal decomposition (POD) methods. On the one hand pointwise (in time) error bounds have been proved in case DQs are added to the set of snapshots [1], and, indeed, counterexamples in [1] show that if DQs are not included, pointwise projection errors degrade with the number of snapshots. On the other hand, while some authors report improvement in their numerical simulations if DQs are included in the data set, others find just the opposite.

In the present talk, we comment on recent results in [2] adding light on why, in agreement with the numerical experience of some authors, it may be possible to obtain good results in practice without including DQs. In particular, we show that if a function has first derivatives (with respect to time) square-integrable in time, POD projection errors do not degrade with the number of snapshots, and that POD methods converge with a rate as close to optimal as the smoothness of the function being approximated allows. We

do this by obtaining discrete versions of Agmon and interpolation inequalities in Sobolev spaces, which allow to bound the L^∞ norm of a function in terms of the L^2 norm and higher-order Sobolev's norms.

References

[1] B. Koc, S. Rubino, M. Schneier, J. Singler and T. Iliescu. On optimal pointwise in time error bounds and difference quotients for the proper orthogonal decomposition. *SIAM J. Numer. Anal.*, 59(4) (2021), 2163–2196.

[2] B. García-Archilla and J. Novo, Pointwise Error Bounds in POD Methods Without Difference Quotients. *J. Sci. Comput.*, 103, 24 (2025). https://doi.org/10.1007/s10915-025-02838-9

Mathematical and Numerical Study for a Bioglass Bioactivity Degradation

A. Hadji *(University of Batna2 Mostefa Benboulaid-Batna, ALGERIA)* & A. Merah & F.Z. Nouri *(Badji Mokhtar University-Annaba, Algeria)*

The development of porous bioactive glasses is part of a multidisciplinary task; where this family of substitutes is particularly adapted to regenerative medicine and suitable for many applications such as prolonged-release drugs. For example in pharmacology, the development of bioactive systems have shown that the release of drugs from the synthesized porous bio-glasses is controlled by a diffusion mechanism, such as a dissolution-precipitation process, due to the porosity criteria. Unfortunately the experimental evaluation of the degradation of bioactive glasses in contact with body fluid requires long-term in vitro tests.

In this work we develop a mathematical model, based on a system of reaction-diffusion equations, to analyse the dissolution and bioactivity for a bio-glass; using simple and low cost numerical schemes. Here we first show the well-posedness of the derived mathematical model, then we propose a numerical framework using adapted numerical schemes to show useful results in real applications.

Recovered finite-element methods for the time-Harmonic Maxwell equations.

Abdalaziz Hamdan & Fillipe Georgiou, Tristan Pryer, Christopher Rowlatt *(University of Bath)*

We present a novel class of recovered finite element methods (R-FEM) for the efficient numerical approximation of the time-harmonic Maxwell equations. This approach combines the benefits of conforming and non-conforming methods by employing discontinuous local approximation spaces and recovery operators to enforce global conformity. We demonstrate the efficacy of the method and validate our theoretical analysis through extensive numerical experiments, showing its potential for solving complex electromagnetic scattering problems.

Uniformly convergent numerical methods for singularly perturbed convection-diffusion problems with interior layers on curvilinear domains

Alan F. Hegarty *(University of Limerick)* & Eugene O'Riordan *(Dublin City University)*

In [1] a finite difference method was constructed to solve singularly perturbed convection-diffusion problems posed on curvilinear domains. Constraints were imposed on the data so that only regular exponential boundary layers appear in the solution. A domain decomposition method was used, comprising a rectangular grid outside the boundary layer and a Shishkin mesh, aligned to the curvature of the outflow boundary, near the boundary layer.

We now wish to examine how this approach works for more general problems, in particular problems with interior layers. Various novel meshes will be examined for such problems.

References

[1] Hegarty, A.F., O'Riordan, E. A numerical method for singularly perturbed convection-diffusion problems posed on smooth domains. J Sci Comput 92, 84 (2022).

Numerical algorithms for nonlinear wave equations via elliptic regularisation.

Brian Hennessy & Lehel Banjai & Emmanuil Georgoulis *(Heriot-Watt University)*

In this talk we present an algorithm for numerically solving nonlinear wave (NLW) equations based on an elliptic regularisation approach conjectured by Ennio De Giorgi. This approach guarantees existence and uniqueness to a solution of a regularised nonlinear wave equation which converge to a solution of NLW, even in cases where the NLW is not well posed.

Using this framework, we design an algorithm for solving the NLW via space-time finite elements which inherits desirable properties of the continuous problem

with particular attention being paid to the time discretisation and stability of the algorithm.

Fast Newton Transform: Interpolation in Downward Closed Polynomial Spaces

Phil-Alexander Hofmann & Damar Wicaksono & Michael Hecht *(CASUS at Helmholtz-Zentrum Dresden-Rossendorf)*

The *Fast Newton Transform* (FNT) addresses the computational bottleneck that arises in solving high-dimensional problems such as 6d Boltzmann, Fokker-Planck, or Vlaslov equations, multi-body Hamiltonian systems, and the inference of governing equations in complex self-organizing systems. Specifically, the challenge lies in numerically computing function expansions and their derivatives fast, while achieving high approximation power. The FNT is a Newton interpolation algorithm with runtime complexity $\mathcal{O}(N\,n\,m)$, where N is the dimension of the downward closed polynomial space, n its degree and m the spatial dimension. We select subgrids from tensorial Leja-ordered Chebyshev-Lobatto grids based on downward-closed sets. This significantly reduces the number of coefficients, $N \ll (n+1)^m$, while achieving optimal geometric approximation rates for a class of analytic functions known as Bos–Levenberg–Trefethen functions. Specifically, we investigate ℓ^p-multi-index sets, where the Euclidean degree ($p = 2$) turns out to be the pivotal choice for mitigating the curse of dimensionality. Furthermore, the differentiation matrices in Newton basis are sparse, enabling the implementation of fast pseudo-spectral methods on flat spaces, polygonal domains, and regular manifolds. Numerical experiments validate the algorithm's superior runtime performance over state-of-the-art approaches.

High-order contour integral methods for strongly continuous operator exponentials

Andrew Horning & Adam R. Gerlach *(Rensselaer Polytechnic Institute)*

Exponential integrators based on contour integral transforms lead to powerful numerical solvers for a variety of ODEs, PDEs, and other time-evolution equations. They are easy to parallelize and lead to global-in-time approximations that can be efficiently evaluated anywhere within a finite time horizon. However, there are theoretical challenges that restrict their use-cases to classes of smooth evolution equations associated with analytic semigroups. In this talk, we show how to use carefully regularized contour integral representations to construct high-order quadrature schemes for the much larger and less regular class of strongly continuous semigroups. Our algorithms are accompanied by explicit high-order error bounds and near-optimal parameter selection. We illustrate the method's attractive features through several PDE examples associated with singular behavior, causality, and non-normality. Along the way, we highlight how simple ideas from semigroup theory can augment traditional techniques in numerical linear algebra to tackle common tensions that arise while computing functions of operators.

Discretising (non-local) Poisson operators with finite elements

James Jackaman *(NTNU)*

In this talk, we introduce a general methodology for discretising Hamiltonian PDEs using finite element methods. Our methodology is constructed such our discretisations exactly conserve the underlying energy (the Hamiltonian functional). We will outline our methodology through designing discretisations of the Korteweg-de Vries equation, before extending it to support the discretisation of nonlocal Poisson structures. This generalisation will lead us to a new discretisation of the Kadomtsev-Petviashvili equation.

Non-Conforming Least Square Spectral Element Method for Elliptic Boundary Layer Problems on Smooth Domains

Sonia Jangra & Akhlaq Husain *(Jamia Millia Islamia)*, Subhashree Mohapatra *(IIIT-Delhi)*

Boundary layers are rapidly varying solution components that arise in singularly perturbed boundary value problems. These layers typically arise in narrow regions near the domain boundary and appear across a wide range of applications. For example, in fluid dynamics, they emerge in the Navier–Stokes equations under small viscosity; in semiconductor device modelling and in structural mechanics, particularly in plate and shell models they arise due to sharp variations near the boundary caused by small boundary layer parameters.

To accurately resolve these layers specially designed numerical methods, particularly those analyzed in appropriate Sobolev norms, are required. Techniques such as layer-adapted meshes, *hp*-FEM, exponential meshes and spectral methods with geometric refinement have been developed to address these challenges.

In this work, we propose a non-conforming least-squares spectral element method for two-dimensional elliptic boundary layer problems in smooth domains. We derive stability estimates and a numerical scheme

based on minimizing a least square functional and prove parameter robust error estimates using p and hp version of the spectral element method. It is shown that the approximation error decays $O\left(W^{-\alpha}\right)$, α is a constant. Numerical results demonstrate that the proposed method robustly captures boundary layers with high accuracy, confirming its effectiveness and stability, even in the presence of sharp solution gradients.

A Nonconforming Least-Squares Spectral Element Method for 2D/3D Stokes Problems with Discontinuous Viscosity and Singular Forces

Shivangi Joshi & Kishore Kumar Naraparaju (*BITS-Pilani Hyderabad Campus, India*) & Subhashree Mohapatra (*IIIT Delhi*)

In this paper, we discuss a least-squares spectral element approach for Stokes flows with singular forces along an interface. The given domain is discretized into a finite number of subdomains so that the division matches along the interface. The interface is resolved exactly using blending elements. The higher-order spectral element functions are used, and they are nonconforming. A suitable least-squares functional is proposed. The interface conditions across the interface are enforced in appropriate Sobolev norms in the minimizing functional. The method is shown to be exponentially accurate, and various numerical examples are presented to validate the theoretical estimates.

A rigorous a posteriori error bound for the Landau–Lifshitz–Gilbert equation

Stefan Karch & Willy Dörfler *(Karlsruhe Institute of Technology)*

Micromagnetic phenomena, such as sharp domain walls, drive the strong interest in adaptive methods for the Landau–Lifshitz–Gilbert (LLG) equation. In this talk, we derive an a posteriori error bound for the discretization error in both time and space for the LLG equation. In the work of Akrivis et al. [AFKL21], optimal-order a priori error estimates for the LLG equation were established using a tangent plane scheme. This 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 handle the nonlinear constraint for the space discretization.

Building upon these results, we extend the analysis of the tangent plane scheme by deriving a rigorous a posteriori error bound for the two-step BDF method with standard higher-order conforming finite elements based on arguments in [BB19]. To establish the a posteriori estimate, we combine the elliptic reconstruction, which allows us to control the spatial errors by standard a posteriori estimators, with the three-point reconstruction in time. By combining these reconstructions, we effectively split the error in both space and time. Finally, we demonstrate in numerical experiments the optimal order of the a posteriori error bounds.

References

[AFKL21] Georgios Akrivis, Michael Feischl, Balázs Kovács, and Christian Lubich. Higher-order linearly implicit full discretization of the Landau-Lifshitz-Gilbert equation. *Math. Comp.*, 90(329):995–1038, 2021.

[BB19] Eberhard Bänsch and Andreas Brenner. A posteriori estimates for the two-step backward differentiation formula and discrete regularity for the time-dependent Stokes equations. *IMA J. Numer. Anal.*, 39(2):713–759, 2019.

Efficiently Learning Instance-Optimal Linear System Solvers

Mikhail Khodak *(Princeton University)*, Edmond Chow, Maria-Florina Balcan & Ameet Talwalkar

The main computational load in many scientific computing tasks, e.g. in the numerical simulation of many partial differential equations, is taken up by the need to solve a long sequence of linear systems. This fundamental task can be accelerated by treating each linear system instance as a data point passed to a lightweight machine learning algorithm that can adaptively set hyperparameters and preconditioners using only the number of iterations as feedback. We propose and analyze several algorithms for doing so, proving that in certain settings they asymptotically (in the length of the sequence of linear systems) select the instance-optimal configuration of successive over-relaxation, an important classical solver often used as a preconditioner in Krylov subspace methods and as a multi-grid smoother. The efficacy of this approach for speeding up numerical simulation is verified in several settings.

Linearized Localized Orthogonal Decomposition for Nonlinear Nonmonotone PDEs

Maher Khrais & Barbara Verfürth *(Universität Bonn)*

In the talk we present a multiscale method for the nonlinear nonmonotone elliptic problem in the framework of the Local orthogonal decomposition (LOD) for solving nonlinear nonmonotone elliptic PDE of the

following form

$$-\nabla \cdot (\alpha(x,u)\nabla u) = f.$$

In particular we present the construction of the problem-adapted multiscale space inspired by the ideas presented in [2] for nonlinear monotone problems. We also present some linearization techniques that can be used to convert the corrector problem into a linear elliptic problem that can be then localized and solved efficiently on the fine scale to define the basis of the new problem-adapted space [1]. We also discuss the elements of a priori error analysis of the method without any structural assumptions on the nonlinear coefficients for instance periodicity or scale separation [3]. We then show some numerical experiments that indicate the criterion for choosing the linearization point, and also elaborate the theoretical results that support the applicability of our numerical approach to non-monotone PDEs e.g., Richards equation.

References

[1] D. Peterseim, *Variational multiscale stabilization and the exponential decay of fine-scale correctors*, Mathematics of Computation, 114 :341–367, 2021.

[2] B. Verfürth, *Numerical homogenization for nonlinear strongly monotone problems*, IMA J. Numer. Anal., 42(2): 1313–1338, 2022.

[3] M. Khrais and B. Verfürth, *Linearized Localized Orthogonal Decomposition for Quasilinear Nonmonotone Elliptic PDE*, arXiv: 2502.13831, URL: https://arxiv.org/abs/2502.13831, 2025.

An overlapping grid spectral collocation analysis on a newly developed hybrid nanofluid flow model

Melusi Khumalo *(University of South Africa)*

The present study investigates the axisymmetric stagnation point radiative flow of a Cu-Al2O3/water hybrid nano-fluid over a radially stretched/shrunk disk. In this paper, a new mathematical model has been developed by taking into consideration the concept of different nanoparticles concentration in a hybrid nanofluid, which are Brownian motion and thermophoresis of nanoparticles. A new model for entropy generation has also been provided in the present study. The non-dimensional governing equations of the developed mathematical model are solved using newly developed and efficient overlapping grid spectral collocation method. Numerical stability and residual error test are provided here to show the accuracy of the numerical method in this mathematical model. The outcomes of fluid flow, temperature, and two different types of concentration profiles are depicted, and described in graphical and tabular forms. For the limiting instances, comparison shows excellent agreement among current and results established in the literature. Increasing the strength of magnetic field is seen to increase the radial component of fluid velocity as well as the entropy generated within the system. Two different nanofluid concentration profiles are increasing and decreasing with rising thermophoresis and Brownian motion parameters, respectively, from a particular height above the disk because of the revised nanofluid boundary condition. Temperature profile increases here with increasing Biot number, and increasing Brinkman number causes higher entropy generation number for both stretching and shrinking disks. The enhanced thermal characteristics of the hybrid nanofluid over the single particle nanofluid has been observed.

Towards Computing Eigenvectors of Tridiagonals to High Relative Accuracy in $O(n^2)$ Time

Plamen Koev & Per-Olof Persson *(San Jose State University & University of California – Berkeley)*

The tridiagonal eigenvalue/eigenvector problem is a central research problem in numerical linear algebra since every symmetric eigenvalue problem reduces to a tridiagonal one first.

Currently to solve a tridiagonal eigenvector problem, one has to make a choice between:

- eigenvectors that are guaranteed to be orthogonal (e.g., via QR iteration), but at $O(n^3)$ cost, or
- an $O(n^2)$ algorithm that does not guarantee orthogonality of the eigenvectors [2, 3].

In this talk we present a new algorithm, which does compute all eigenvectors of a tridiagonal matrix to high relative accuracy via the corresponding singular value problem of the bidiagonal Cholesky factor. Our algorithm is more accurate than that of Demmel [1] and does complete the computation of the eigenvector matrix, albeit in *factored* form, in $O(n^2)$ time.

Despite depending on only $O(n)$ parameters and being represented as a product of $O(n^2)$ Givens rotations, computing the eigenvector matrix in $O(n^2)$ has eluded the researchers for over three decades. We will address the structure that this matrix possesses (such as doubly lowerly totally positive and polynomial Vandermonde) as well as possible approaches to its fast computation.

References

[1] J. Demmel, *Accurate singular value decompositions of structured matrices*, SIAM J. Matrix Anal. Appl. **21** (1999), no. 2, 562–580.

[2] Inderjit S. Dhillon, Beresford N. Parlett, and Christof Vömel, *Glued matrices and the MRRR algorithm*, SIAM J. Sci. Comput. **27** (2005), no. 2, 496–510.

[3] Ming Gu and Stanley C. Eisenstat, *A divide-and-conquer algorithm for the symmetric tridiagonal eigenproblem*, SIAM J. Matrix Anal. Appl. **16** (1995), no. 1, 172–191.

A posteriori error analysis for Cahn–Hilliard on a bulk-surface with dynamic boundary conditions.

Michael Lantelme & Nils Bullerjahn *(Paderborn University)*

We will discuss the a posteriori error analysis of bulk-surface Cahn–Hilliard systems with dynamic boundary conditions. The differential equation is approximated with linear finite elements in space and backward Euler method in time. The presented derivation allows to attain a reliable error indicator capturing the error of the approximation including the contributions from the boundary conditions and geometric contributions from the discretization of the bulk-surface. Brief insights on the implementation of an adaptive algorithm based on the indicators are presented.

Numerical experiments complement the theory and highlight the benefits of using adaptive methods.

Surrogate modelling for sparse parameter- and time-dependent data

Robin Lautenschlager *(University of Stuttgart)*

Complex multi-X models are common in many scientific fields. These simulations are often computationally expensive, dependent on certain model parameters and in particular highly time-dependent.

This holds in particular for inverse problems. Here the complex forward models have to be executed repeatedly for varying inputs, resulting in the ability to identify problem specific model parameters.

Surrogate modelling has great potential in this setting. Replacing the fully resolved complex multi-X model with a faster and less complex surrogate, by simultaneously retaining the characteristics of the underlying model, can lead to an enormous speed up of the simulation and significantly increases the usability of the model in real-world scenarios.

In this talk, we consider a data-driven surrogate model approach derived from various basic machine learning regression methods. Polynomial Chaos Expansion motivates the discretization and decoupling of model parameters and time for the training procedure. The model itself is founded on the theories of Graph Neural Networks, because the basic idea is that outputs are not only obtained from the input data points itself but also from information inherited from surrounding points in the parameter-time domain. Additionally the surrogate has to be stable for training on sparse data, because the procurement of training data from the complex multi-X model is still very costly.

We discuss and compare effectiveness and applicability of these approaches for the societally relevant setting of AMI amputation surgery. This is aan upcoming limb amputation technique, where the residual muscles of an agonist-antagonist pair are (re-)connected via a tendon in order to restore their mechanical and neural interaction.

The nonconforming locking-free virtual element method for the poroelasticity model

Hao Liang *(Katholische Universität Eichstätt-Ingolstadt)* & Hongxing Rui *(Shandong University)*

The poroelasticity model describes the coupled phenomena of porous media deformation and internal fluid flow. It has been extensively developed and widely applied in various engineering fields, including biomedical engineering, petroleum engineering, and medicine. Numerous studies have focused on numerical methods for the poroelasticity model, with particular attention to addressing nonphysical pressure oscillations and Poisson locking in numerical solutions. These issues often arise in cases of nearly incompressible materials, low permeability, or small-time steps at the start of the consolidation process.

To overcome these issues, we proposed and analyzed a locking-free nonconforming virtual element method for the three-field poroelasticity model, encompassing displacements, Darcy velocity, and pore-pressure. We showed the well-posedness and derived optimal error estimates for the discrete schemes. Numerical experiments confirmed the convergence analysis and demonstrated that our method effectively avoids Poisson locking and nonphysical pressure oscillations.

Building on the virtual element method, this approach is both versatile and adaptable to general polygonal

meshes. Furthermore, by incorporating the reconstruction method, this approach is extended to incompressible poroelasticity models.

References

[1] H. Liang, H. X. Rui, The nonconforming locking-free virtual element method for the Biot's consolidation model in poroelasticity, Comput. Math. Appl., 148 (2023) 269-281.

[2] H. Liang, H. X. Rui, A parameter robust reconstruction nonconforming virtual element method for the incompressible poroelasticity model, Appl. Numer. Math., 202 (2024) 127-142.

Pauli matrices: a better basis for relativistic electrodynamics?

Ben McKeon & Alan Hegarty *(University of Limerick)*

In the four-vector formalism of special relativity, the translation and rotation operators used to construct Lorentz transformations do not commute. As a result, using four-vectors as a basis when creating numerical methods for charged particle dynamics causes substantial, intrinsic errors. Moreover, these errors are further amplified in the strong electromagnetic fields of high-power lasers and compact stellar objects, where particle velocities may approach the speed of light.

However, by taking advantage of the isomorphism $\mathbb{R}^4 \to \mathbb{C}^{2\times 2}$, it is possible to construct numerical methods which are unaffected by noncommuting operators by using the Pauli matrices as a basis. Nevertheless, the time evolution of such methods typically takes place in the comoving frame of each particle, making their implementation computationally expensive for a large ensemble of particles.

In this work, using the composition method of Yoshida, we extend to fourth order a method previously considered by Gordon and Hafizi. Specifically, we consider the effect of converting from the comoving frame of the particle to a common laboratory frame and the ability of our method to preserve phase space volume. Furthermore, in numerical experiments, we compare our method with an explicit leapfrog method of Hairer, Lubich and Shi and also the standard methods of Boris, Vay and Higuera and Cary. Finally, we briefly discuss further extensions of numerical methods constructed using a Pauli matrix basis.

References

Gordon, D.F. and Hafizi, B., 2021. Special unitary particle pusher for extreme fields. *Computer Physics Communications, 258*, p.107628.

Yoshida, H., 1990. Construction of higher order symplectic integrators. *Physics letters A, 150*(5-7), pp.262-268.

Hairer, E., Lubich, C. and Shi, Y., 2023. Leapfrog methods for relativistic charged-particle dynamics. *SIAM Journal on Numerical Analysis, 61*(6), pp.2844-2858.

Boris, J.P., 1970. Relativistic plasma simulation-optimization of a hybrid code. In *Proc. Fourth Conf. Num. Sim. Plasmas* (pp. 3-67).

Vay, J.L., 2008. Simulation of beams or plasmas crossing at relativistic velocity. *Physics of Plasmas, 15*(5).

Higuera, A.V. and Cary, J.R., 2017. Structure-preserving second-order integration of relativistic charged particle trajectories in electromagnetic fields. *Physics of Plasmas, 24*(5).

Numerical Convergence of the Regularised Immersed Boundary Method

Alexandre X. Milewski & Charles S. Peskin *(CIMS)*

Developed in 1972, the immersed boundary method has since been used as a means to simulate fluid-membrane interactions. However, whilst the numerical convergence of such a method has been empirically verified, it is theoretically unproven due to the singular forcing terms present in the governing equations. In this talk, I introduce a variant of the immersed boundary method that deals with co-dimension 2 surfaces in a Navier-Stokes fluid (the co-dimension being defined as the dimension of the fluid minus the dimension of the boundary) and demonstrate that it is numerically convergent in theory as well as in practice.

Convergence rates of curved boundary element methods for the 3D Helmholtz equation

Hadrien Montanelli, Luiz Faria & Pierre Marchand *(Inria)*

We present improved convergence rates for boundary element methods on curved geometries, applied to the 3D Helmholtz equation with smooth data. Our analysis is based on sharp consistency estimates for the perturbed sesquilinear forms arising in the discretization. We support our theoretical results with 3D nu-

merical experiments using polynomial basis functions and curved triangular elements of up to fourth order.

References

[1] A. S. Sznitman. Topics in propagation of chaos. In *Hennequin, P.-L. (ed.) École d'Été de Probabilités de Saint-Flour XIX - 1989. Lecture Notes in Mathematics*, **vol. 1464**, Springer, Berlin, Heidelberg, 1991.

[2] T. Breiten, K. Kunisch, and L. Pfeiffer. Control strategies for the Fokker–Planck equation. *ESAIM: Control, Optimisation and Calculus of Variations*, **24**(2):741-763, 2017.

Mixed finite element approximation for non-divergence form elliptic equations with random input data

Amireh Mousavi (*Friedrich Schiller University Jena*)

We study an elliptic partial differential equation in non-divergence form with both a random diffusion matrix and a random forcing term. To approximate its solution, we propose a hybrid numerical method: a mixed-type continuous finite element discretization in the physical domain, combined with a stochastic collocation method.

At the continuous level, we introduce a stochastic cost functional, which is later modified to directly incorporate the vanishing tangential trace condition through a mesh-dependent formulation. This allows us to avoid enforcing the constraint within the function space itself. A mesh-dependent norm is defined, and an accompanying error analysis is provided.

In the stochastic domain, we apply a collocation scheme based on the zeros of suitable tensor-product orthogonal polynomials. This results in a set of uncoupled deterministic problems, enabling efficient parallel computation.

Finally, we present an a priori error estimate for the fully discrete scheme and demonstrate convergence with respect to the discretization parameters. Numerical experiments confirm the theoretical predictions.

A robust preconditioner for saddle-point problems in an industrial context

Michaël Ndjinga & Pierre-Loïc BACQ *(Université Paris-Saclay)*

We consider the linear resolution of saddle-point systems arising from the discretisation of coupled or constrained systems. In many cases, such systems are challenging to solve by iterative methods and the developments of efficient preconditioners is an active field of research [1]. In this presentation, we present a robust block-preconditioner for a 2×2 block-system of the form

$$\begin{pmatrix} A & B^T \\ B & -C \end{pmatrix}, \tag{1}$$

with A a symmetric positive definite (SPD) block, and C positive semi-definite. Such problems have been extensively studied especially in academic communities and different families of preconditioners have been proposed [2]. In this talk, we highlight a problematic that has not been much investigated to the extent of our knowledge. In an industrial context, theoretical hypotheses are often not satisfied. Even the most simple systems of the form of Equation (1) can become challenging to solve for state-of-the-art linear solvers when the diagonal dominance of the block A is lost. Such a difficulty occurs for instance on distorted meshes. Industrial solvers then resort to direct solvers with all the ensuing limitations.

In order to tackle this difficulty, we present a new algebraic preconditioner [4] with increased robustness for systems such as Equation (1). The key idea involves an algebraic transformation of the system that compensates the loss of diagonal dominance. Since the approach we propose is algebraic in nature, it can be applied to a broad class of problems. In the context of the talk, we focus on systems encountered during the resolution of the incompressible Navier-Stokes equations discretised on large unstructured meshes with the PolyMAC scheme [3, 4].

The talk will first highlight the loss of robustness of classical approaches when considering distorted meshes. In a second time, we describe our innovative preconditioner based on an algebraic transformation of the linear system based on an approximate block LU decomposition. Numerical results show impressive convergence on problems of industrial complexity and good parallel scalability.

References

[1] M. Benzi, G. H. Golub, J. Liesen. *Numerical Solution of Saddle Point Problems.* Acta Numerica, 14, 1–137, 2005. doi :10.1017/S0962492904000212.

[2] M. Benzi, A. J. Wathen. *Some Preconditioning Techniques for Saddle Point Problems*, pp. 195–211. Springer Berlin Heidelberg, Berlin, Heidelberg, 2008. doi :10.1007/978-3-540-78841-6_10.

[3] P.-L. Bacq, A. Gerschenfeld, M. Ndjinga. *PolyMAC : Staggered Finite Volume Methods on General*

Meshes for Incompressible Navier–Stokes Problems. In E. Franck, J. Fuhrmann, V. Michel-Dansac, L. Navoret, eds., *Finite Volumes for Complex Applications X—Volume 1, Elliptic and Parabolic Problems*, pp. 149–156. Springer Nature Switzerland, Cham, 2023.

[4] Bacq, P.-L., Gerschenfeld, A. and Ndjinga, M. (2025), PolyMAC: A Staggered Finite Volume Method on General Meshes for Incompressible Navier-Stokes Equations. Int J Numer Meth Fluids. https://doi.org/10.1002/fld.5398

Computing the spectrum of the Schrödinger equation with quasiperiodic potential

Jitse Niesen *(University of Leeds)*

We want to compute the eigenvalues and eigenstates of the Schrödinger equation with a quasiperiodic potential, e.g., $V(x) = \cos(x) + \cos(\tau x)$ where τ is irrational. This is motivated by quasicrystals, in which the atoms are well-ordered but not arranged in a periodic pattern. The eigenstates in spatially periodic crystals is governed by Bloch theory, but the corresponding theory for quasicrystals is still in its infancy.

There are many numerical methods for computing the eigenstates of the Schrödinger equation with a periodic potential. However, they assume either that the potential is periodic or that the eigenstates are localized. We will discuss a spectral method based on the Fourier–Bohr expansion, which uses a basis of quasiperiodic functions. Numerical results suggest that this method is well suited to approximate eigenstates that extend over the entire real line. We will compare the numerical results with theorems from functional analysis, which state that part of the spectrum may be dense but not continuous and another part may be a Cantor set.

Mathematical Modeling and Simulation for Multiphase Flows

Fatma Zohra Nouri *(Badji Mokhtar University-Annaba)*

A persistent theme throughout the study of multiphase flows is the need to model and predict their detailed behavior and the phenomena that they manifest. The latest developments in mutiphase flow combine a powerhouse of theoretical, analytical, and numerical methods to create stronger verification and validation modeling methods. Such models are explored, experimentally through equipped laboratory-sized models, theoretically using mathematical equations, or numerically exploiting the power of computers to study the complexity of the flow.

Here, we exploit mathematical and numerical analysis for multiphase flows in problems derived from hydrogeology and medicine, where we consider simultaneous flow of materials with different states or phases [1, 3] or materials with different chemical properties but in the same state/phase [2, 4].

References

[1] M. Albert-Gimeno, I. Hadji, T. Joshi, L. Kimpton, T. Kwan, G. Lang, S. Moise, S. Naire, F.Z. Nouri, G. Richardson & R. Whittaker, Targeting stem cells following I.V. injection using magnetic particle based approaches, Mathematics in Medecine 2012.

[2] A. Assala, N. Djedaidi & F.Z. Nouri, Dynamical behaviour of miscibles fluids in Porous Media, Int. J. Dynamical Systems and Differential Equations, Vol. 8, No.3, 2018, 176-188.

[3] Cuc Bui, Vanessa Lleras & Olivier Pantz, Modélisation et simulation de la dynamique des globules, hal.archives 2015.

[4] F.Z. Nouri and N. Djedaidi, Interface Dynamics for a Bi-Phasic Problem in Heterogeneous Porous Media, Dynamics of Continuous, Discrete and Impulsive Systems Series B: Applications & Algorithms 30 (2023) 21-33.

Optimal bounds for POD approximations of infinite horizon control problems based on time derivatives

Julia Novo & Javier de Frutos & Bosco García-Archilla *(Universidad Autónoma de Madrid)*

In this talk we consider the numerical approximation of infinite horizon problems via the dynamic programming approach. The value function of the problem solves a Hamilton-Jacobi-Bellman (HJB) equation that is approximated by a fully discrete method. It is known that the numerical problem is difficult to handle by the so called curse of dimensionality. To mitigate this issue we apply a reduction of the order by means of a new proper orthogonal decomposition (POD) method based on time derivatives. We carry out the error analysis of the method using recently proved optimal bounds for the fully discrete approximations. Moreover, the use of snapshots based on time derivatives allow us to bound some terms of the error that could not be bounded in a standard POD approach. Some numerical experiments show the good performance of the method in practice.
Let $D \subset\subset \mathbb{R}^d$ be a d-dimensional domain with com-

pact closure. We consider the approximation of the $d_0 < d$ dimensional zero level-set $\mathcal{L}_0 := \{x \in \bar{D} : f(x) = 0\}$ where the Lipschitz function f is either accessible directly or when $f(x) = \mathbb{E}\left[\tilde{f}(x)\right]$ for all $x \in \bar{D}$. Given an approximation scheme with a priori error bounds and L^p bounds on the $\tilde{f}$-approximation error, we propose a grid-based adaptive sampling scheme which produces an approximation to $\mathcal{L}_0$ with expected cost-complexity reduction of $\varepsilon^{\left(\frac{p+d-d_0}{\alpha p}\right)}$ compared to a non-adaptive scheme, where α is the known convergence rate of an interpolation scheme. We provide the numerical analysis and extensive experiments to show that these rates hold in practice.

Adaptivity in PDE-Constrained Optimal Control

Jenny Power & Tristan Pryer *(University of Bath)*

Optimal control problems (OCPs) constrained by partial differential equations (PDEs) are fundamental in various scientific and engineering applications, including fluid dynamics and radiotherapy treatment planning. To ensure well-posedness, such problems typically require regularisation involving a small regularisation parameter. The resulting OCP is equivalent to solving a singularly perturbed PDE. In this talk we will discuss adaptive strategies for PDE-constrained control problems discretised by Galerkin finite element methods (FEMs). This includes adaptive mesh-refinement guided by robust a posteriori error estimates, and adaptive regularisation where the regularisation parameter is allowed to vary elementwise [1].

References

[1] Jenny Power and Tristan Pryer. *"Adaptive regularisation for PDE-constrained optimal control"*. Journal of Computational and Applied Mathematics (2025). DOI:https://doi.org/10.1016/j.cam.2025.116651.

Maxey-Riley-Gatignol Equations for Tracking Lagrangian Devices in Chemical Reactors

Vamika Rathi & Daniel Ruprecht *(Hamburg Institute of Technology)*

The Maxey-Riley-Gatignol equations (MaRGe) are used to describe the motion of small, spherical inertial particles in fluids. They model the movement of inertial particles in a wide range of environmental, industrial, and geophysical processes, such as the dispersion of the COVID-19 virus, movement of particles in chemical reactors, and cloud formation. MaRGe are integro-differential equations due to the presence of the history force term, which is an integral over the full time interval over which the particle moves, that makes them difficult and computationally expensive to solve. Most researchers neglect the history force; however, studies show that the term has a significant effect not only on the trajectories of individual particles but also on their larger-scale Lagrangian dynamics.

In my talk, I will present a numerical solver for the 3D MaRGe using the quadrature schemes for solving the history term and Adams-Bashforth methods for solving the full equations as proposed by Daitche (2013). For verification, I will derive an analytical solution using techniques from the paper by Candelier et. al. (2004) for a 3D vortex as test case. Finally, I will show results where we attempt to track simulated as well as experimental particles using filtering algorithms, modified to use a simplified version of MaRGe as prediction model instead of the commonly used assumption of constant acceleration over a time step.

Data-driven discovery of chemical reaction networks

Abraham Reyes-Velazquez & Stefan Güttel & Jonas Latz & Igor Larrosa *(University of Manchester)*

Automatic discovery of chemical reaction networks (CRNs) from data is a central challenge in chemical kinetics. While recent methods like SINDy can recover governing equations, they are insufficient for identifying chemically valid network structures. In this talk, we present a general framework for the automatic and complete discovery of closed CRNs from time-series data, recovering both the dynamical system and a plausible reaction graph consistent with mass-action kinetics.

CLASSIX beyond the Euclidean norm

Kaustubh Roy & Stefan Guettel *(University of Manchester)*

The CLASSIX algorithm is a fast and explainable approach to data clustering. In its original form, this method utilizes the first principal component of the data matrix to truncate the search for nearby data points, using the Cauchy-Schwarz inequality, with proximity being defined in terms of the Euclidean distance. In this work, we demonstrate methods to extend CLASSIX to other distance measures by showcasing its effectiveness in the Manhattan distance and the Tanimoto distance. CLASSIX in these two distance metrics uses the 1-norm of the data vectors as the sorting criterion. The triangle inequality is used

as a general search termination criterion applicable to any p-norm, and the Baldi intersection inequality is used as a search truncation criterion for the Tanimoto distance.

Error analysis of splitting methods for 3D semilinear wave equations with finite-energy solutions

Maximilian Ruff *(Karlsruhe Institute of Technology)*

We study splitting schemes for the time integration of the 3D energy-(sub)critical semilinear wave equation on the full space and the torus under the finite-energy condition. In the case of a cubic nonlinearity, we show that a filtered Strang splitting converges with almost second order in L^2 and almost first order in H^1. If the nonlinearity has a quartic form instead, we show an analogous convergence result with an order reduced by $1/2$. For the energy-critical quintic nonlinearity, we show first-order convergence in L^2 for the filtered Lie and Strang splittings. To our knowledge these are the best convergence results available for the 3D semilinear wave equation under the finite-energy condition and they include the first error analysis performed for a scaling-critical problem. Our approach relies on continuous- and discrete-time Strichartz estimates. Dispersive estimates in discrete time were already used in the context of semilinear Schrödinger equations by Ignat, Ostermann, Schratz, and others. We also make use of the integration and summation by parts formulas to exploit cancellations in the error terms. Moreover, in the torus case, error bounds for a full discretization using the Fourier pseudo-spectral method in space are given. Finally, we discuss a numerical example indicating the sharpness of our theoretical results. This is partially joint work with Roland Schnaubelt (Karlsruhe).

Asymptotic and numerical approximations to the zeros of parabolic cylinder functions

Diego Ruiz-Antolín & T. Mark Dunster, Amparo Gil, Javier Segura *(Universidad de Cantabria)*

The zeros of parabolic cylinder functions have numerous applications in science and engineering. They are used, for example, in the analysis of fluid flow in cylindrical channels and in the scattering of electromagnetic waves at parabolic boundaries.

In this talk, we present uniform asymptotic approximations for the real and complex zeros of the parabolic cylinder function $U(a, z)$, involving certain combinations of the zeros of Airy functions [1]. The expansions are valid for a large in absolute value (whether positive or negative), and uniformly for unbounded z (real or complex).

The accuracy of the approximations for the complex zeros is tested using a method (implemented in Maple) for finding the complex zeros of solutions of second-order ODEs [2]. A fixed-precision implementation of this method for parabolic cylinder functions will also be discussed in the talk. The numerical algorithm incorporates, among other techniques, Taylor series and Liouville-Green expansions of U(a,z) and its derivative in the region where the zeros are located [3].

References

[1] T.M. Dunster, A. Gil, D. Ruiz-Antolín, J. Segura. Uniform asymptotic expansions for the zeros of parabolic cylinder functions. Stud. Appl. Math. 154 (2025) e70004.

[2] J. Segura. Computing the complex zeros of special functions. Numer. Math. 124 (4) (2013) 723-752.

[3] T.M. Dunster, A. Gil, D. Ruiz-Antolín, J. Segura. A numerical algorithm for computing the zeros of parabolic cylinder functions in the complex plane. Submitted.

More on Nonnegative Tucker Decompositions

Subhayan Saha & Giovanni Barbarino & Nicolas Gillis *(Université de Mons)*

This contribution aims to dig deeper into nonnegative Tucker decompositions (nTDs), and is complementary to the contribution "Nonnegative Tucker Decomposition: Introduction, Identifiability and Algorithms" by N. Gillis. I will cover in more details identifiability and algorithmic issues of nTDs, and illustrate them on various numerical experiments. The abstract of our paper is as follows: Tensor decompositions have become a central tool in data science, with applications in areas such as data analysis, signal processing, and machine learning. A key property of many tensor decompositions, such as the canonical polyadic decomposition, is identifiability, that is, the factors are unique, up to trivial scaling and permutation ambiguities. This allows one to recover the groundtruth sources that generated the data. The Tucker decomposition (TD) is a central and widely used tensor decomposition model. However, it is in general not identifiable. In this talk, we first introduce and motivate matrix and tensor decomposition models, with a focus on nonnegative matrix factorization (NMF) and nonnegative Tucker decomposition (NTD). Then, we study the identifiability of NTD. For order-2 tensors, that is, matrices, NTD

is equivalent to a nonnegative tri-factorization model. By adapting and extending identifiability results of NMF, we provide uniqueness results for order-2 NTD. The conditions require the nonnegative matrix factors to have some degree of sparsity, namely satisfy the sufficiently scattered condition, while the core matrix only needs to be full rank. We extend the result to order-3 tensors, which requires the nonnegative matrix factors to satisfy the same sufficiently scattered condition, while the core tensor only needs to have some slices (or linear combinations of them) or unfoldings with full column rank. We also discuss how this result can be extended to higher-order tensors. Finally, we propose an efficient algorithm to compute these unique NTDs, which we illustrate on synthetic and real data.

Goal-oriented adaptive stochastic collocation finite element method for PDEs with log-normal parametrisation of coefficients

Andrey Savinov & Alex Bespalov *(University of Birmingham)*

In this talk, we present a general goal-oriented adaptive strategy for approximating quantities of interest (QoIs) derived from solutions to PDEs with random inputs. We focus on the case where PDE coefficients are log-normal random fields that depend on a countable number of uncertain parameters. The QoIs are defined in terms of bounded linear or continuously Gâteaux differentiable nonlinear functionals. To compute the approximations, we employ the sparse grid stochastic collocation finite element method (SC-FEM).

Our adaptive strategy is driven by new, reliable a posteriori error estimates specifically tailored to QoIs. We follow the idea proposed in [1] and include a correction term in the QoI approximation in order to compensate for the lack of global Galerkin orthogonality in the SC-FEM setting. Furthermore, the developed algorithm adaptively activates uncertain parameters in the PDE coefficient and performs adaptive spatial and parametric refinements. We will discuss theoretical foundations of the algorithm, including the introduction of auxiliary Gaussian measures, as well as the procedure for activating modes/parameters in the PDE coefficient and an effective strategy for generating collocation points in the unbounded parameter domain.

We will demonstrate the performance of the adaptive algorithm for a range of linear and nonlinear goal functionals by presenting computational results for a representative elliptic problem with log-normal parametric coefficient.

References

[1] A. Bespalov, D. Praetorius, T. Round, and A. Savinov, Goal-oriented error estimation and adaptivity for stochastic collocation FEM, *SIAM/ASA J. Uncertain. Quantif.*, 2025 (to appear; preprint is available on arXiv:2406.05028).

An extrapolated and provably convergent algorithm for nonlinear matrix decomposition with the ReLU function

Giovanni Seraghiti & Nicolas Gillis, Margherita Porcelli *(University of Mons / University of Florence)*

In this talk, we discuss the following nonlinear matrix decomposition (NMD) problem: given a matrix X, find a low-rank matrix WH such that $X \approx f(WH)$, where $f(WH)$ applies the scalar function f elementwise on WH. We focus on the case where X is sparse and nonnegative, and $f(\cdot) = \max(0, \cdot)$, the rectified linear unit (ReLU) nonlinear activation. The corresponding low-rank decomposition is referred to as ReLU decomposition.

We first provide the intuition behind ReLU decomposition and its connection with neural networks. As a motivation, we show examples of applications in data compression, manifold learning, and matrix completion with entries missing not at random.

Then, we focus on how to compute ReLU decompositions, presenting different problem formulations and state-of-the-art algorithms that one can use to solve them. In particular, we consider the minimization of $\|Z - WH\|_F^2$, where $X = \max(0, Z)$, that is a nonconvex problem in three variables W, H, and Z, referred to as three-block-ReLU-NMD (3B-ReLU-NMD). To address the 3B-ReLU-NMD problem, we propose a new extrapolated block coordinate descent (eBCD-NMD) algorithm that converges under mild assumptions.

We conclude by illustrating numerical experiments on various applications, showing that eBCD-NMD performs well against the state-of-the-art on synthetic and real-world data sets.

A posteriori error analysis of hybrid high order method for elliptic obstacle problem

Ritesh Singla *(IMAG, University of Montpellier)* & Kamana Porwal *(Indian Institute of Technology Delhi)*

The obstacle problem is a fundamental mathematical model that arises in various fields of mathematics, en-

gineering, physics, and economics, having a wide ranging applications. In mathematical terms, the problem seeks a function that minimizes a certain energy functional and remains on or above the obstacle function. In this work, a posteriori error analysis of the elliptic obstacle problem is addressed using hybrid high-order methods. The method involve cell unknowns represented by constant polynomials and face unknowns represented by degree-s polynomials, where $s \in \{0, 1\}$. The discrete obstacle constraints are specifically applied to the cell unknowns. The analysis hinges on the construction of a suitable Lagrange multiplier, a residual functional and a linear averaging map. The reliability and the efficiency of the proposed a posteriori error estimator is discussed, and the study is concluded by numerical experiments.

Finite element approximations of a micromagnetic model at elevated temperatures

Agus Soenjaya & Beniamin Goldys, Kim-Ngan Le, Thanh Tran *(University of New South Wales)*

The (deterministic or stochastic) Landau–Lifshitz–Bloch (LLB) equation is a vector-valued nonlinear (S)PDE that arises in micromagnetism, modeling the time evolution of magnetisation in ferromagnetic materials at elevated temperatures. In this talk, I will present and analyse some fully discrete finite element schemes for the LLB equation. Under suitable regularity assumptions on the exact solution, optimal order of convergence results are obtained for these schemes. In the stochastic case, additional regularisation procedures are employed, partly due to the lack of known regularity of solutions in $d \geq 2$.

This talk is based in part on joint work with Beniamin Goldys (University of Sydney), Kim-Ngan Le (Monash University), and Thanh Tran (UNSW).

Nodally bound-preserving discontinuous Galerkin methods for charge transport

Alex Trenam & Gabriel R. Barrenechea & Tristan Pryer *(Heriot–Watt University)*

Ensuring the positivity of density variables is not only important for solutions to remain physically-relevant, but it can also be a crucial factor in the stability of coupled systems describing charge transport. In this talk I will discuss recent work developing discontinuous Galerkin methods for the time-dependent drift–diffusion equation and the coupled Poisson–Nernst–Planck model, which describe the evolution of charged particle concentrations in the presence of a global electric field. The methods in question preserve the positivity (or rather non-negativity) of the charge densities at the Lagrange nodes, and the discretisation of the coupled system uses the natural energy framework to derive stability without any time step restriction.

A tailored, matrix free interior point method for fast optimization on gas networks

Rowan Turner & Lars Schewe & John Pearson *(University of Edinburgh)*

We consider a PDE-constrained optimization problem arising from the prospective use of hydrogen as an energy carrier to support fully renewable electric grids. One important question is whether existing natural gas infrastructure can be reused for hydrogen to this end, and the challenges this brings for the control of these networks. We expect that a hydrogen network which uses gas generated from excess renewable electricity would be more difficult to control as the patterns of injection and withdrawal would be much less regular than today. Additional challenges arise from new operating parameters required for hydrogen – such as controlling for pressure fluctuations to prevent pipe-ageing. Motivated by a need for instationary optimization methods on networks at scale, we present a specialized, matrix free interior point method for gas problems. Our test problem is a linepack optimization problem using a discretization of the 1d isothermal Euler equations, as a step towards understanding the important questions above. By incorporating a bespoke preconditioned iterative solver to tackle the linearized systems at each iteration of the interior point method, which form the key computational bottleneck in such a method, we utilize the highly structured nature of the problem to gain efficiency. The expectation is that the method will scale well with both network size and time windows, and be generalizable to broader PDE-constrained network optimization problems.

Error Estimates for a Linear Fully-Discrete Finite Element Scheme for the Ferromagnetic Magnetohydrodynamical Model

Noah Vinod *(UNSW)* & Thanh Tran *(UNSW)*

Ferromagnetic magnetohydrodynamics concerns the study of conducting fluids with intrinsic magnetisation under the influence of a magnetic field. It is a generalisation of the magnetohydrodynamical equations and takes into account the dynamics of the magnetisation of a fluid. First proposed by Lingam [1], the usual equations of magnetohydrodynamics, namely the Navier-Stokes equation and the induction equation, are coupled with the Landau-Lifshitz equation. Theoretical discussions related to the well-posedness of solutions to this coupled system have been carried out

in the past [2], but no rigorous numerical study has been conducted. Here, we discuss the error estimates for a linearised finite element scheme that uses continuous piecewise polynomial finite elements. The error estimates are developed using induction and the pointwise constraint for the Landau-Lifshitz equation is achieved asymptotically.

References

[1] Lingam, M., 2015. Dissipative effects in magneto-hydrodynamical models with intrinsic magnetization. Communications in Nonlinear Science and Numerical Simulation 28, 223–231.

[2] Vinod, N., Tran, T., 2024. Well-Posedness for a Magnetohydrodynamical Model with Intrinsic Magnetisation. arXiv.

Fast Macaulay Null Space

Raphaël Widdershoven & Nithin Govindarajan & Lieven De Lathauwer *(KU Leuven)*

Finding the roots of systems of multivariate polynomial equations is a fundamental problem with broad applications across science and engineering. A widely used class of methods for solving such systems is based on Macaulay matrices—large, multi-level quasi-Toeplitz matrices that encode the system's algebraic structure. The roots can be obtained from their null space, but computing this null space is often the primary computational bottleneck due to the large size of these Macaulay matrices.

We present a new method that leverages the nested structure of the Macaulay matrices to avoid constructing the full matrix. It achieves substantial gains in both memory and computation time. For quadratic systems in N variables, this strategy reduces the overall complexity from approximately $\mathcal{O}(2^{6N})$ to $\mathcal{O}(2^{4N})$. For $N = 8$, runtime drops from 600 seconds to just 4 seconds.

Crucially, we show that all operations involved in constructing the Macaulay matrix can be performed directly within its null space. This perspective opens new possibilities for efficient algorithm design in polynomial system solving and beyond.

Convergence of Calderón residuals

Anouk Wisse *(Delft University of Technology)*, Ralf Hiptmair & Carolina Urzúa-Torres

Convergence rates for Galerkin discretizations of boundary integral equations are usually available in fractional and sometimes even negative order spaces. Because of this, when one wishes to debug a BEM code, one chooses a reference solution and typically uses some of the Galerkin matrices to measure the error. In other words, one exploits the norm equivalence between the solution space of the boundary integral equation and the energy norm of the operator. However, this method only works if the implementation of the Galerkin matrices is done correctly, which can be hard to verify.

In this talk, we present a tool to validate the implementation of boundary integral operators that circumvents this problem. To do this, we compute expected convergence rates for residuals based on the Calderón identities for general differential operators. These rates can be used to validate the implementation of boundary integral operators. Our estimates are in standard infinity and Euclidean vector norms, thus avoiding the use of hard-to-compute norms. We illustrate this with two examples: the Laplacian and time-harmonic Maxwell's equations. For implementation we use the software package Bempp (`https://bempp.com/`).