29th Biennial Conference on Numerical Analysis

27 – 30 June, 2023

Contents

Nothing in here

Invited Speakers

Coralia Cartis	University of Oxford	cartis@maths.ox.ac.uk
Lars Eldén	Linköping University	lars.elden@liu.se
Emmanuil Georgoulis	Heriot-Watt University & NTU Athens	e.georgoulis@hw.ac.uk
Chen Grieff	University of British Columbia	greif@cs.ubc.ca
Laura Grigori	EPFL and PSI, Switzerland	laura.grigori@epfl.ch
Angela Kunoth	University of Cologne	kunoth@math.uni-koeln.de
Sven Leyffer	Argonne National Laboratory	leyffer@anl.gov
Ricardo Nochetto	University of Maryland	rhn@math.umd.edu
Daniel Peterseim	University of Augsburg	daniel.peterseim@uni-a.de
Gabriel Peyre	DMA, École Normale Supérieure	gabriel.peyre@ens.fr
Catherine Powell	University of Manchester	catherine.powell@manchester.ac.uk
Christiane Tretter	University of Bern	tretter@math.unibe.ch

Abstracts of Invited Talks

Dimensionality reduction techniques for nonconvex optimization

Coralia Cartis *(University of Oxford)*

Modern applications such as machine learning involve the solution of huge scale nonconvex optimization problems, sometimes with special structure. Motivated by these challenges, we investigate more generally, dimensionality reduction techniques in the variable/parameter domain for local and global optimization that rely crucially on random projections. We describe and use sketching results that allow efficient projections to low dimensions while preserving useful properties, as well as other tools from random matrix theory and conic integral geometry. We focus on functions with low effective dimensionality, a common occurrence in applications involving overparameterized models and that can serve as an insightful proxy for the training landscape in neural networks. We obtain algorithms that scale well with problem dimension, allow inaccurate information and biased noise, have adaptive parameters and benefit from high-probability complexity guarantees and almost sure convergence.

Multiway Spectral Graph Partitioning: Cut Functions, Cheeger Inequalities, and a Simple Algorithm

Lars Eldén *(Linköping University)*

The problem of multiway partitioning of an undirected graph is considered. A spectral method is used, where the $k > 2$ largest eigenvalues of the normalized adjacency matrix (equivalently, the k smallest eigenvalues of the normalized graph Laplacian) are computed. It is shown that the information necessary for partitioning is contained in the subspace spanned by the k eigenvectors. The partitioning is encoded in a matrix Ψ in indicator form, which is computed by approximating the eigenvector matrix by a product of Ψ and an orthogonal matrix. A measure of the distance of a graph to being k-partitionable is defined, as well as two cut (cost) functions, for which Cheeger inequalities are proved; thus the relation between the eigenvalue and partitioning problems is established. Numerical examples are given that demonstrate that the partitioning algorithm is efficient and robust.

hp-Version discontinuous Galerkin methods on essentially arbitrarily-shaped elements

Emmanuil Georgoulis *(University of Leicester)*

We extend the applicability of the popular interior-penalty discontinuous Galerkin (dG) method discretizing advection-diffusion-reaction problems to meshes comprising of extremely general, essentially arbitrarily-shaped element shapes. In particular, our analysis allows for curved element shapes, arising, *without* the use of (iso-)parametric elemental maps. The feasibility of the method relies on the definition of a suitable choice of the discontinuity-penalization parameter, which turns out to be essentially independent on the particular element shape. A priori error bounds for the resulting method are given under very mild structural assumptions restricting the magnitude of the local curvature of element boundaries. Numerical experiments are also presented, indicating the practicality of the proposed approach. This work generalizes our earlier work detailed in the monograph [A.Cangiani, Z.Dong, E.H. Georgoulis and P.Houston, *hp*-version discontinuous Galerkin methods on polygonal and polyhedral meshes, SpringerBriefs in Mathematics, Springer, Cham, 2017] from polygonal/polyhedral meshes to essentially arbitrary element shapes involving curved faces without imposing any additional mesh conditions.

The talk is based on joint work with A. Cangiani (Nottingham) and Z. Dong (INRIA, Paris).

Numerical Solution of Double Saddle-Point Systems

Chen Greif *(University of British Columbia)*

Double saddle-point systems are drawing increasing attention in the past few years, due to the importance of associated applications and the challenge in developing efficient numerical solvers. In this talk we describe some of their numerical properties and make some distinctions between this family and the more well-established class of classical 2-by-2 block-structured saddle-point systems. We derive eigenvalues bounds, expressed in terms of extremal eigenvalues and singular values of block sub-matrices. The analysis includes bounds for preconditioned matrices based on block diagonal preconditioners using Schur complements, and it is shown that in this case the eigenvalues are clustered within a few intervals bounded away from zero. Analysis for approximations of Schur complements is included. We illustrate some of the

numerical challenges and our findings on a Marker-and-Cell discretization of the Stokes-Darcy equations.

Randomization techniques for solving large scale linear algebra problems

Laura Grigori *(EPFL and PSI, Switzerland)*

This talk will discuss several recent advances in using randomization and communication avoiding techniques for solving large scale linear algebra problems. We first consider solving linear systems of equations and discuss in this context a randomized Gram-Schmidt process for orthogonalizing a set of vectors. We show that this process is as efficient as classical Gram-Schmidt and numerically stable as modified Gram-Schmidt,
while also exploiting mixed precision. The usage of randomization in Krylov subspace methods as GMRES or FOM is further discussed. We then introduce a block orthogonalization method in the context of solving eigenvalue problems and discuss its numerical behaviour.

Adaptive Approximations for PDE-Constrained Parabolic Control Problems

Angela Kunoth *(University of Cologne)*

Numerical solvers for PDEs have matured over the past decades in efficiency, largely due to the development of sophisticated algorithms based on closely intertwining theory with numerical analysis. Consequently, systems of PDEs as they arise from optimization problems with PDE constraints also have become more and more tractable.

Optimization problems constrained by a parabolic evolution PDE are challenging from a computational point of view: They require to solve a system of PDEs coupled globally in time and space. For their solution, time-stepping methods quickly reach their limitations due to the enormous demand for storage. An alternative approach is a full space-time weak formulation of the parabolic PDE which allows one to treat the constraining PDE as an operator equation without distinction of the time and space variables. An optimization problem constrained by a parabolic PDE in full space-time weak form leads to a coupled system of corresponding operator equations which is, of course, still coupled globally in space and time.

For the numerical solution of such coupled PDE systems, adaptive methods appear to be most promising, as they aim at distributing the available degrees of freedom in an a-posteriori-fashion to capture singularities in the data or domain. Employing wavelet schemes, we can prove convergence and optimal complexity. The theoretical basis for proving convergence and optimality of wavelet-based algorithms for such type of coupled PDEs is nonlinear approximation theory and the characterization of solutions of PDEs in Besov spaces.

Wavelet schemes are, however, more involved when it comes to implementations compared to finite element approximations. I will finally address corresponding ideas and results.

Topological Design Problems and Integer Optimization

Sven Leyffer *(Argonne National Laboratory)*

Topological design problems arise in many important manufacturing and scientific applications, including additive manufacturing and the design of electromagnetic cloaks. We formulate these problems as mixed-integer PDE-constrained optimization problems (MIPDECOs), and we show that despite their seemingly hopeless complexity, MIPDECOs can be solved efficiently. We present two classes of scalable algorithms. The first class of methods is based on solving the continuous relaxation (a PDE-constrained optimization problem), and uses clever rounding techniques. We outline the convergence behavior of this approach, and show that we can obtain an integer solution whose objective value is arbitrarily close to the continuous relaxation. The second class of methods extends trust-region methods for nonlinear optimization, and we show that this class converges under mesh-refinement. We illustrate these solution techniques with examples from topology optimization.

Liquid Crystal Polymeric Networks: Modeling, Approximation, and Computation

Ricardo H. Nochetto *(University of Maryland)*

Liquid crystal polymeric networks (LCNs) are materials where a nematic liquid crystal is coupled with a rubbery material. When actuated with heat or light, the interaction of the liquid crystal with the rubber creates complex shapes. Thin bodies of LCNs are natural candidates for soft robotics applications. Starting from the classical 3D trace energy formula of Bladon, Warner and Terentjev (1994), we derive a 2D membrane energy as the formal asymptotic limit of the

3D energy and characterize the zero energy deformations. The membrane energy lacks convexity properties, which lead to challenges for the design of a sound numerical method. We discretize the problem with conforming piecewise linear finite elements and add a higher order bending energy regularization to address the lack of convexity. We prove that minimizers of the discrete energy converge to zero energy states of the membrane energy in the spirit of Gamma convergence; this includes the presence of creases. We solve the discrete minimization problem via an energy stable gradient flow scheme. We present computations showing the geometric effects that arise from liquid crystal defects as well as computations of nonisometric origami, both within and beyond theory. This work is joint with L. Bouck and S. Yang.

Multiscale methods for operator compression and surrogate learning

Daniel Peterseim *(University of Augsburg)*

The talk deals with the efficient approximation of coefficient-to-surrogate maps in the general framework of multi-scale PDEs parameterised by strongly heterogeneous coefficient fields. The surrogate models are represented by sparse, problem-adapted bases that emerged from modern numerical homogenisation methods. They aim to reduce complex large-scale problems to effective models at a given target scale of interest, taking into account the effects of features at unresolved scales. Sparsity is preserved by localisation strategies that enforce a (super-)exponential decay of basis functions relative to their discretisation scales. We will discuss multi-resolution variants as well as the emulation of local finite element assembly structures within a neural network enhanced learning of coefficient-to-surrogate maps. The collection of illustrative numerical examples includes diffusion problems with random coefficients, nonlinear eigenvalue problems under disorder, and evolution equations.

This work is part of the project *Computational Random Multiscale Problems* (Grant agreement No. 865751) that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme.

Scaling Optimal Transport for High dimensional Learning

Gabriel Peyré *(DMA, École Normale Supérieure)*

Optimal transport (OT) has recently gained a lot of interest in machine learning. It is a natural tool to compare in a geometrically faithful way probability distributions. It finds applications in both supervised learning (using geometric loss functions) and unsupervised learning (to perform generative model fitting). OT is however plagued by the curse of dimensionality, since it might require a number of samples which grows exponentially with the dimension. In this talk, I will explain how to leverage entropic regularization methods to define computationally efficient loss functions, approximating OT with a better sample complexity. More information and references can be found on the website of our book "Computational Optimal Transport" `https://optimaltransport.github.io/`.

How and Why to be Intrusive

Catherine E. Powell *(University of Manchester)*

In engineering applications (heat transfer, fluid flow, elasticity etc), we often encounter physics-based models consisting of partial differential equations (PDEs) with uncertain inputs, which are reformulated as so-called parametric PDEs. In the field of Uncertainty Quantification (UQ), we typically model uncertain inputs as random variables. Given a probability distribution for the inputs, the forward UQ problem then consists of trying to estimate statistical quantities of interest related to the model solution. Conversely, given (usually, noisy) data relating to the model solution, the inverse UQ problem consists of trying to infer the uncertain inputs themselves.

Over the last two decades, a myriad of numerical schemes have been developed in the numerical analysis community to tackle forward and inverse UQ problems involving PDEs. The vast majority of these are sampling schemes and are non-intrusive in the sense that users do not have to modify existing solvers and codes for the associated deterministic PDEs. This is very attractive in industrial settings. Stochastic Galerkin methods, also known as intrusive polynomial chaos methods, standard apart and are much less widely used in practice. Key challenges include: how to design the Galerkin approximation space, and how to solve the associated linear systems of equations. In this talk, I will outline the intrusive approach for forward UQ in PDE models, its advantages and limitations, and emphasise the importance of **adaptivity**.

Challenges for non-selfadjoint spectral problems in analysis and computation

Christiane Tretter *(University of Bern)*

Non-selfadjoint spectral problems appear frequently in a wide range of applications. Reliable information about their spectra is therefore crucial, yet extremely difficult to obtain. This talk focuses on tools to master these challenges such as spectral pollution or spectral invisibility. In particular, the concept of essential numerical range for unbounded linear operators is introduced and studied, including possible equivalent characterizations and perturbation results. Compared to the bounded case, new interesting phenomena arise which are illustrated by some striking examples. A key feature of the essential numerical range is that it captures, in a unified and minimal way, spectral pollution which may affect e.g. spectral approximations of PDEs by projection methods or domain truncation methods. As an application, Maxwell's equations with conductivity will be considered.

(Joint work with S. Bögli, M. Marletta, and also F. Ferraresso)

Minisymposia abstracts

Minisymposium M1

Multiscale and Polytopal Discretisation Methods for Complicated Domains and Heterogeneous Structures
Organisers
Zhaonan Dong and Roland Maier

Offline-online strategy for multiscale problems with random perturbations

Barbara Verfürth *(University of Bonn)* & Axel Malqvist

Modern tailor-made materials with enhanced properties, so-called metamaterials, typically consist of periodic arrangement of composites. This leads to multiscale problems, where the coefficients of the PDE vary on small spatial scales. When investigating the robustness of the material properties under imperfections and fabrication faults, one can model this by adding certain random perturbations to the underlying multiscale coefficient.

In this talk, we propose a numerical strategy [1] to efficiently compute approximate solutions of the multiscale problem in a multi-query context, i.e., for many different realizations of the random perturbations. The key idea is to pre-compute the local stiffness matrices of the used numerical multiscale method for a set of carefully selected coefficients. For any queried realization, these are combined to a low-dimensional global matrix in an efficient manner. This offline-online strategy reduces the computational effort in comparison to classical multiscale methods, where new multiscale basis functions and stiffness matrices have to be computed for each realization. We justify our technique by error bounds as well as extensive numerical tests.

References

[1.] A. Malqvist, B. Verfürth. An offline-online strategy for multiscale problems with random defects. *ESAIM Math. Model. Numer. Anal.,* 56(1):237–260, 2022.

Hybrid discontinuous Galerkin methods on multiple levels

Andreas Rupp & Guido Kanschat & Peipei Lu & Roland Maier *(LUT University)*

Hybrid finite element schemes approximate the trace of an unknown solution to a partial differential equation on the mesh skeleton (the union of the faces in a mesh). Afterward, these schemes use this trace approximation to recover the primal and dual unknowns. This strategy has several advantages over standard finite elements, such as an enhanced order of convergence, smaller symmetric positive systems of linear equations, and preservation of physically meaningful quantities.

Virtually all of the available multilevel (multigrid and multiscale) techniques for finite elements exploit the fact that their test and trial spaces are nested. However, the test and trial spaces are not nested for hybrid finite elements because their main approximate lives on the mesh's skeleton, which grows with refinement. Thus, the major obstacle that blocks the way to practical multigrid methods comprises the construction of stable mesh transfer operators. Several recent works have addressed this issue by exchanging the hybrid formulation for a non-hybrid formulation in a preliminary step. Afterward, these approaches use the available multilevel strategies for non-hybrid finite elements.

We proceed differently and preserve the advantageous properties of hybrid finite elements on all mesh levels. To this end, we devise stable mesh transfer operators and provide relevant convergence results for our hybrid, multilevel finite elements. This approach allows us to use identical discretizations on all mesh levels (homogeneous strategy) instead of the heterogeneous methods that use different discretizations on different mesh levels.

Super-localized numerical homogenization

Moritz Hauck *(University of Augsburg)* & Daniel Peterseim (University of Augsburg)

The objective of numerical homogenization is to provide an accurate and efficiently computable approximation of the solution space of partial differential operators, even when the coefficients are arbitrarily rough and non-periodic. A common technique for constructing such approximate solution spaces is to apply the solution operator to classical finite element spaces.

However, the canonical basis functions of these spaces typically decay slowly and are therefore intractable in practice. In this talk, we introduce the Super-Localized Orthogonal Decomposition [M. Hauck, D. Peterseim, *Math. Comp. 92 (2023), 981-1003*], which identifies near-local basis functions, resulting in a particularly efficient numerical homogenization method. Furthermore, we demonstrate the application of the method beyond elliptic homogenization problems, as well as a recent modification of the method with improved stability properties for high-contrast channeled coefficients.

A Multiscale Hybrid Method

Gabriel R. Barrenechea *(University of Strathclyde)*

In this talk I will present the Multiscale Hybrid (MH) method recently proposed in [2]. The method is built as a close relative to the Multiscale Hybrid Mixed (MHM) method ([1, 3]), but with the fundamental difference that a novel definition of the Lagrange multiplier is introduced. The practical implication of this is that both the local problems to compute the basis functions, as well as the global problem, are elliptic, as opposed to the MHM method (and also other previous methods) where a mixed global problem is solved, and constrained local problems are solved to compute the local basis functions. The error analysis of the method is based on a hybrid formulation, and a static condensation process is done at the discrete level, so the final global system only involves the Lagrange multipliers. We test the performance of the method by means of numerical experiments for problems with multiscale coefficients, on general polygonal meshes, and we carry out comparisons with the MHM method in terms of performance, accuracy, and memory requirements.

The work presented in this talk was done in collaboration with Antonio Tadeu A. Gomes (LNCC, Petropolis, Brazil), and Diego Paredes (Universidad de Concepción, Chile).

References

[1.] R. Araya, Ch. Harder, D. Paredes, and F. Valentin, Multiscale hybrid mixed method. SIAM Journal on Numerical Analysis, **51** (6), 3505–3531, (2013).

[2.] G.R. Barrenechea, A.T. Gomes, and D. Paredes, A multiscale hybrid method. Preprint hal-03907060v2, (2022).

[3.] G.R. Barrenechea, F. Jaillet, D. Paredes, and F. Valentin, The multiscale hybrid mixed method in general polygonal meshes. Numerische Mathematik **145**(1), 197–237, (2020).

Superconvergence of a multiscale method for ground state computations of Bose-Einstein condensates

Anna Persson & Patrick Henning *(Uppsala University)*

To compute ground states of Bose-Einstein condensates the stationary Gross-Pitaevskii equation (GPE) is often used. In this talk we revisit a two-level multiscale technique introduced in (P. Henning, A. Mal qvist, and D. Peterseim, *SIAM J. Numer. Anal.* 52, 2014) for computing numerical approximations to the GPE. The method is based on localized orthogonal decomposition of the solution space, which exhibit high approximation properties and improves the convergence rates compared to classical finite element methods. This reduces the computational cost for computing the ground states significantly.

In the original paper, high order convergence of the method was proven, but even higher orders were observed numerically. In this talk we show how to improve the analysis to achieve the observed rates, which are as high as $O(H^6)$ for the eigenvalues. We also show some numerical experiments for both smooth and discontinuous potentials.

Furthermore, when Bose-Einstein condensates are rotated (or stirred) a number of quantized vortices typically appears. This is one of many interesting properties that such condensates exhibit. We shall discuss and give an outlook on how to model this phenomenon efficiently by designing appropriate solution spaces.

Frequency-explicit analysis of a multiscale finite element method to approximate scattering by highly heterogeneous obstacles

Théophile Chaumont-Frelet & Z. Kassali *(Inria Université Côte d'Azur)*, E.A. Spence *(University of Bath)*

I will consider the scattering of acoustic waves by a penetrable obstacle featuring a highly heterogeneous structure. Under suitable assumptions on the shape of the obstacle and its microstructure, I will first present new stability estimates for the Helmholtz problem with fully-explicit constants that grow polynomially as the

frequency increases. In the second part of the talk, I will introduce a multiscale hybrid-mixed (MHM) method to numerically approximate the solution. In particular, I will present a priori error estimates that are explicit in the frequency, the microstructure characteristic size, the polynomial degree, and the mesh size.

A mixed-dimensional fracture mechanics model based on the linear theory of the Cosserat continuum

Omar Durán & Jan Martin Nordbotten & Inga Berre & Eirik Keilegavlen *(University of Bergen)*

The research presented here is an extension of the linearized mixed-dimensional poromechanical model for fractured media presented in [1]. There is a discussion of classical continuum mechanics in terms of finite and infinitesimal strains. In this study, we consider the linear theory of Cosserat's (micropolar, asymmetric) continuum as a different perspective on fracture mechanics. The continuum theory of Cosserat is a multiscale continuum. When the characteristic length scale of heterogeneities (the periodicity size) is comparable to the Cosserat intrinsic lengths, then the effective medium is a Cauchy continuum, whereas when the intrinsic length of the Cosserat is larger (and comparable to the domain size), then the effective medium is a Cosserat medium [2]. Our study addresses the second-order form of the equations with the HHO discretization and presents numerical results.

References

[1] W.M. Boon and J.M. Nordbotten. "Mixed-dimensional poromechanical models of fractured porous media". In: Acta Mechanica 234.3 (Dec. 2022), pp. 1121–1168. doi: 10.1007/s00707- 022-03378-1.

[2] D. Ammosov et al. "Generalized macroscale model for Cosserat elasticity using Generalized Multiscale Finite Element Method". In: Journal of Computational Physics 461 (2022), p. 111011. issn: 0021-9991. doi: https://doi.org/10.1016/j.jcp.2022.111011.

Isoparametric Virtual Element Methods

Harry Wells & Andreas Dedner & Matthew Hubbard & **Andrea Cangiani** *(SISSA)*

The Virtual Element Method (VEM) is well known to provide flexible approximations on general polygonal and polyhedral meshes, including with curved elements. This generality gives a clear advantage in the approximation of PDE problems posed on moving domains as meshes may remain acceptable under deformation and topological change. This motivation has prompted, on the one hand, numerous extensions of the VEM with curved elements and, on the other, the development of virtual element methods for time-dependent and transformed domains. We propose a tool which sits in between such developments by extending to the VEM the classical theory of isoparametric finite elements for the solution of elliptic PDEs. The idea is to construct a virtual element space on a (static) mesh which is itself virtual in the sense that it is obtained via virtual element maps. The approach is based on bespoke polynomial approximation operators to construct a computable method. A priori analysis proves that the optimal rate of convergence can be achieved. Numerical experiments implemented using the DUNE-VEM platform confirm the optimal rate of convergence. We envisage our analysis as a first step towards a rigorous treatment of problems posed on time-dependent domains and surface PDEs.

A posteriori error estimates for discontinuous Galerkin methods and hybrid high-order methods on polygonal and polyhedral meshes

Zhaonan Dong *(Inria Paris & École des Pont)* & Andrea Cangiani *(SISSA)* & Alexandre Ern *(École des Pont & Inria Paris)* & Emmanuil Georgoulis *(Heriot-Watt University & National Technical University of Athens)* & Géraldine Pichot *(Inria Paris & École des Pont)*

We present a new residual-type energy-norm a posteriori error analysis for discontinuous Galerkin (dG) and hybrid high-order (HHO) methods for elliptic problems. The new error bounds are also applicable to dG and HHO methods on meshes consisting of elements with very general polygonal/polyhedral shapes. The case of simplicial and/or box-type elements is included in the analysis as a special case. In particular, for the upper bounds, an arbitrary number of very small faces is allowed on each polygonal/polyhedral element as long as certain mild shape regularity assumptions are satisfied, which is essential for designing the adaptive algorithms based on the mesh agglomeration strategy for large-scale simulations. As a corollary, the present analysis holds for meshes with an arbitrary number of irregular hanging nodes per element. The proof hinges on a new conforming recovery strategy in conjunction with a Helmholtz decomposition formula. Local lower bounds are also proven for a number of practical cases. Several academic numerical experiments are presented to highlight the practical value of the derived a posteriori error bounds as error estimators and also the

flexibility of the adaptive algorithms based on mesh agglomeration.

Space–time virtual elements: a priori error analysis, residual error estimators, and adaptivity

Lorenzo Mascotto & Sergio Gómez & Andrea Moiola & Ilaria Perugia *(University of Milano-Bicocca)*

We present a space–time virtual element method for parabolic problems based on a standard Petrov-Galerkin formulation. Trial and test spaces are nonforming in space, so as to allow for a unified analysis in any spatial dimension. The information between time slabs is transmitted by means of upwind terms involving polynomial projections of the discrete functions. After discussing a priori error estimates, we validate them on some numerical examples and compare the results with those of conforming space–time finite elements.

Moreover, we introduce and assess numerically several properties of a residual-type error estimator: we verify its reliability and efficiency for h-adaptive refinements; compare the performance of the space–time nonconforming virtual and conforming finite element methods; investigate the quasi-efficiency of the error estimator for p- and hp-refinements.

Minisymposium M2

Recent Advances in computational PDEs for uncertainty quantification

Organisers
Alex Bespalov and Michele Ruggeri

Uncertainty Quantification for the Helmholtz equation

Ivan Graham *(University of Bath)*

I'll discuss waves in random media governed by the frequency domain Helmholtz equation, where the coefficients of the PDE (e.g. refractive index) are para metrized random fields, and one wants to compute expected values, or other moments, of quantities derived from the PDE solutions. This leads to the computation of (possibly high-dimensional) integrals in parameter space.

In the high-frequency case, solutions of the PDE are oscillatory in space and (it turns out) also oscillate at the same scale in parameter space. Thus methods designed to deal with the high-dimensionality of the integrals (such as Quasi-Monte Carlo methods) may suffer from degradation in accuracy as the frequency increases.

We provide an insight into this behaviour by looking at a 1D model random Helmholtz problem at high frequency, with refractive index parametrized by (possibly many) uniformly distributed random variables. In this case a hybrid numerical-asymptotic analysis allows us to isolate explicitly the oscillatory components of the solution, and then to show that the expectation of the solution can be written in terms of high-dimensional oscillatory integrals with linear (but possibly variable) phase.

Accordingly we briefly present a new Filon-Clenshaw-Curtis-Smolyak rule capable of computing these integrals (for moderate dimensions) with accuracy which improves as the frequency increases and give a brief numerical illustration.

Most of the talk is joint work with Zhizhang Wu, Dingjiong Ma and Zhiwen Zhang of the University of Hong Kong.

Isogeometric analysis of rough random acoustic scattering

Michael Multerer & Jürgen Dölz, Wei Huang *(Università della Svizzera italiana)*

We study the numerical solution of forward time-harmonic acoustic scattering problems by rough randomly deformed obstacles in three-dimensional space using a fast isogeometric boundary element method. As in [1], realisations of the random scatterer can efficiently be computed by simply updating the NURBS mappings which represent the scatterer. However, unlike [1], we consider a rough random deformation field on the boundary determined by an identity expectation and a covariance operator with slowly decaying eigenvalues. Employing samplets, cp. [2], for the compression of the covariance operator, we use the Cholesky decomposition with nested dissection reordering to obtain a representation of the deformation field. Due to the slow decay of the covariance operator's eigenvalues, higher order quadrature methods for the computation of quantities of interest, such as the scattered wave's expectation and correlation in free space via an artificial, fixed interface enclosing the random obstacle, are not indicated. Therefore, we resort

to the multilevel Monte Carlo method. Numerical results for the forward problem validate the proposed approach.

References

[1.] J. Dölz, H. Harbrecht, C. Jerez-Hanckes, M. Multerer (2022). *Isogeometric multilevel quadrature for forward and inverse random acoustic scattering.* Computer Methods in Applied Mechanics and Engineering, 388, 114242.

[2.] H. Harbrecht, M. Multerer (2022). *Samplets: Construction and scattered data compression.* Journal of Computational Physics, 471, 111616.

Sparse grid approximation of stochastic dynamic micromagnetics

Andrea Scaglioni & Michael Feischl *(TU Wien)*

The Landau–Lifschitz–Gilbert equation is a well established nonlinear PDE model in dynamic micromagnetics, the study of magnetic materials at submicrometer scale. The effect of random thermal fluctuations on the magnetization can be modelled by a *stochastic* generalization of the Landau–Lifschitz–Gilbert problem, a nonlinear SPDE model. To approximate the random solution, we first convert the SPDE to a PDE with parametric coefficients using the Doss-Sussmann transformation and the Lèvy-Ciesielsky parametrization of the Brownian motion. We introduce a new technique to prove analytic regularity of the parameter-to-solution map, a task made challenging by the fact that the problem is nonlinear and the parameters set is not compact. This regularity result is applied to the convergence study of a piecewise-polynomial sparse grid approximation. If time permits, we discuss space and time discretization and multilevel strategies for large-scale simulation.

Error estimation and adaptivity for stochastic collocation finite elements

David Silvester *(University of Manchester)*

A multilevel adaptive refinement strategy for solving linear elliptic partial differential equations with random data is discussed herein. The strategy extends the a posteriori error estimation framework introduced by Guignard & Nobile in 2018 to cover problems with a *nonaffine* parametric coefficient dependence. A suboptimal, but nonetheless reliable and convenient implementation of the strategy involves approximation of the decoupled PDE problems with a common finite element approximation space. Computational results obtained using such a *single-level* strategy are presented in this talk. Results obtained using a potentially more efficient *multilevel* approximation strategy, where meshes are individually tailored, are discussed in a follow-up paper. The codes used to generate the numerical results are available on GitHub.

This is joint work with Alex Bespalov and Feng Xu.

Goal-oriented adaptivity for stochastic collocation finite element methods

Thomas Round [1] & Alex Bespalov [1] & Dirk Praetorius [2] [1] *(University of Birmingham)* [2] *(Vienna University of Technology)*

Finite element methods are often used to compute approximations to solutions of problems involving partial differential equations (PDEs). More recently, various techniques involving finite element methods have been utilised to solve PDE problems with parametric or uncertain inputs. One such technique is the stochastic collocation finite element method, a sampling based approach which yields approximations that are represented by a finite series expansion in terms of a parameter-dependent polynomial basis.

In this talk we address the topic of goal-oriented strategies in the context of the stochastic collocation finite element method. These strategies are used to approximate quantities of interest associated with solutions to PDEs with parameter dependent inputs. First, we follow the ideas in [1], [2] to estimate approximation errors for the corresponding primal and dual problems, use products of these estimates in an adaptive algorithm for approximating quantities of interest, and demonstrate the utility of the proposed algorithm using numerical examples. We will then consider an alternative goal-oriented adaptive strategy based on the dual-weighted residual method for estimating the errors in the quantity of interest.

References

[1.] A. Bespalov, D. Silvester and F. Xu, Error estimation and adaptivity for stochastic collocation finite elements Part I: single-level approximation, *SIAM J. Sci. Comput.*, 44, pp. A3393–A3412, 2022.

[2.] A. Bespalov and D. Silvester, Error estimation and adaptivity for stochastic collocation finite elements Part II: multilevel approximation, *SIAM J. Sci. Com-*

put., 45, pp. A784–A800, 2023.

Adaptive cross sampling approximation to solutions of parametric PDEs

Sergey Dolgov & Robert Scheichl *(University of Bath)*

Partial differential equations with random coefficients constitute an important uncertainty quantification task and a challenging high-dimensional problem. It has been approached with many techniques, such as Monte Carlo, Sparse Grids, Reduced Basis and low-rank tensor decompositions. The latter two offer potentially a lower complexity by finding a tailored low-rank solution approximation. However, generic low-rank algorithms, such as Alternating Least Squares (ALS), can fill-in the sparsity of the original stiffness matrix. As a result, realistic scenarios with fine unstructured grids and large ranks resisted direct treatment with these algorithms. We propose to combine the ALS steps for the spatial variables and the cross approximation steps for the other (e.g. random) variables. This scheme preserves the sparsity (in fact, block-diagonality) of the matrix and allows it to reuse dedicated solvers for the deterministic problem. We show that the new algorithm can be significantly faster than the Sparse Grids and Quasi Monte Carlo methods for smooth random coefficients. Moreover, thus precomputed low-rank tensor surrogate of the entire solution of the forward problem can significantly accelerate Bayesian inference in the inverse problem.

Forward uncertainty quantification with locally supported basis functions

Laura Scarabosio & Wouter van Harten *(Radboud University)*

We consider, as a model problem, a Poisson equation where the diffusion coefficient and the right-hand side depend *nonlinearly* on a random field. The random field is modeled via a Karhunen-Loève expansion where the uncertain parameters are images of uniformly distributed random variables. We are interested in approximating the map from the uncertain parameters to the PDE solution.

Motivated by the results in [1] and [2] for the affine and lognormal case respectively, we show that using basis functions with localized support to model the random field leads to polynomial approximations to the parameter-to-solution map which converge faster than when using globally supported basis functions.

As a particular case, we apply the results to shape uncertainty quantification, where the random field corresponds to the boundary of a star-shaped domain on which the PDE is defined. Here, the motivation for using functions with localized support might not reside only in higher computational efficiency, but also, from a modeling point of view, in having more geometrical flexibility in describing shape variations.

References

[1.] Bachmayr, M., Cohen, A., & Migliorati, G. (2017). Sparse polynomial approximation of parametric elliptic PDEs. Part I: affine coefficients. *ESAIM: Mathematical Modelling and Numerical Analysis*, 51(1), 321-339.

[2.] Bachmayr, M., Cohen, A., DeVore, R., & Migliorati, G. (2017). Sparse polynomial approximation of parametric elliptic PDEs. Part II: lognormal coefficients. *ESAIM: Mathematical Modelling and Numerical Analysis*, 51(1), 341-363.

Multilevel Monte Carlo Methods with Smoothing

Anastasia Istratuca & Aretha Teckentrup *(University of Edinburgh, Maxwell Institute Graduate School)*

We consider the computational efficiency of Monte Carlo (MC) and Multilevel Monte Carlo (MLMC) methods applied to partial differential equations with random coefficients. These models arise, for example, in groundwater flow modelling, where a common configuration for the unknown parameter is a random field. Further, we make use of the circulant embedding procedure for sampling from the aforementioned coefficient. Then, to further improve the computational complexity of the MLMC estimator, we devise and implement the smoothing technique integrated into the circulant embedding method. This allows us to choose the coarsest mesh on the first level of MLMC independently of the correlation length of the covariance function of the random field, leading to considerable savings in computational cost. We illustrate this with numerical experiments, where we consider different correlation lengths for the random parameter.

Approximating nonlinear quantities of interest using adaptive multilevel stochastic Galerkin FEM

Alex Bespalov[1] & Dirk Praetorius[2] & Michele

Ruggeri [3] [1] *(University of Birmingham)* [2] *(Vienna University of Technology)* [3] *(University of Strathclyde)*

We will discuss the numerical approximation of quantities of interest that target specific features of the solutions to elliptic partial differential equations (PDEs) with parametric or uncertain inputs. We consider a class of elliptic PDEs where the underlying differential operator has affine dependence on a countably infinite number of uncertain parameters. Our focus in this talk is on estimating the propagation of uncertainty to a quantity of interest represented by a *nonlinear* functional of the solution. We present a goal-oriented adaptive algorithm driven by computable estimates of the energy errors in multilevel stochastic Galerkin approximations of the primal and dual solutions. We will discuss recent convergence results for the proposed adaptive algorithm [1] and demonstrate its performance in numerical experiments.

References

[1.] A. Bespalov, D. Praetorius, and M. Ruggeri, Goal-oriented adaptive multilevel stochastic Galerkin FEM, *Preprint*, arXiv:2208.09388, 2022.

Minisymposium M3

Novel discretisation and solution methods for wave propagation problems
Organisers
Théophile Chaumont-Frelet and Victorita Dolean

Using the H-GenEO Coarse Space for Efficient Solution of the Helmholtz equation

Mark Fry & Victorita Dolean & Matthias Langer *(University of Strathclyde)* & Ivan Graham *(University of Bath)*

The Helmholtz equation is a widely used model in wave propagation and scattering problems. However, its numerical solution can be computationally expensive due to its high-frequency oscillations and the potential for a large contrast in coefficients. Parallel domain decomposition methods have been identified as promising solvers for such problems, but they often require a suitable coarse space to achieve robust behaviour.

In this talk, we present the H-GenEO coarse space, which is based on the Generalized Eigenvalue Problem in the Overlap (GenEO). The H-GenEO method constructs an effective coarse space using localized eigenvectors of the Helmholtz operator which can be implemented using various discretization techniques. While the GenEO coarse space is designed for symmetric positive definite problems, the theory cannot be applied to the H-GenEO coarse space due to the indefinite nature of the underlying problem. During this talk it will be shown that the H-GenEO coarse space is capable of providing the required robust behaviour when used with a suitable domain decomposition method.

Numerical experiments in wave propagation problems demonstrate the efficacy of the H-GenEO method, which offers significant computational savings while maintaining high accuracy compared to other methods when applied to the indefinite Helmholtz equation. The results indicate that the H-GenEO coarse space has potential as an efficient tool for solving complex Helmholtz problems, with potential applications in various scientific and engineering domains.

References

[1.] N. Spillane, V. Dolean, P. Hauret, F. Nataf, C. Pechstein, and R. Scheichl. *Abstract Robust Coarse Spaces for Systems of PDEs via Generalized Eigenproblems in the Overlaps.* Numerische Mathematik, 126(4):741–770, 2014.

[2.] N. Bootland, V. Dolean, I. G. Graham, C. Ma, and R. Scheichl. *Overlapping Schwarz methods with GenEO coarse spaces for indefinite and nonself-adjoint problems.* IMA Journal of Numerical Analysis, 08 2022.

A hybridizable discontinuous Galerkin method with characteristic variables for Helmholtz problems

Axel Modave *(POEMS, CNRS, Inria, ENSTA Paris, Institut Polytechnique de Paris, France)* & Théophile Chaumont-Frelet *(Université Côte d'Azur, Inria, CNRS, LJAD, France)*

A new hybridization procedure will be presented for discontinuous Galerkin (DG) discretizations of high-frequency Helmholtz problems. In contrast to standard hybridizable discontinuous Galerkin (HDG) schemes that employ a numerical trace as a Lagrange multiplier, this new approach called CHDG utilizes characteristic variables.

This new choice of auxiliary unknown changes the

properties of the reduced system, which exhibits a structure similar to specific optimized substructuring domain decomposition methods and ultra weak Trefftz formulations. In particular, a simple fixed point iteration always converges to solve the CHDG reduced linear system, which is not the case for standard DG and HDG schemes.

Numerical results will be presented to compare different iterative procedures including fixed point, GMRES and CGNR iterations on 2D benchmarks. On all the considered test cases, the number of iterations is reduced for CHDG as compared to DG and HDG, often by a large amount. Interestingly, the CGNR iteration (which is often disregarded) converges nearly as fast as the GMRES iteration without restart for the CHDG system.

Stable Trefftz approximation of Helmholtz solutions using evanescent plane waves

Emile Parolin *(Inria Paris)* & Nicola Galante, Daan Huybrechs, Andrea Moiola

Solutions u of the Helmholtz equation, $-\Delta u - \kappa^2 u = 0$ with wavenumber $\kappa > 0$, are known to be well approximated by superpositions of propagative plane waves, $\mathbf{x} \mapsto e^{\imath\kappa \mathbf{d}\cdot\mathbf{x}}$, with a real-valued propagation vector $\mathbf{d} \in \mathbb{R}^n$, $n \in \{2, 3\}$. This observation is the foundation of successful Trefftz methods, which are a class of numerical methods that construct approximations in the form of piecewise linear combinations of particular solutions of the equation under consideration, allowing it to get better rates of convergence compared to multipurpose polynomial spaces. However, when too many plane waves are used, the computation of the expansion is known to be numerically unstable, from the quasi linear dependence of plane waves with similar directions of propagation. In fact, we prove that exponentially large coefficients in the expansion are unavoidable in some situations and we explain how this causes numerical instability, which drastically limits the efficiency of the approach in practice.

We recently proved that all Helmholtz solutions in the unit ball in $\mathbb{R}^n$, $n \in \{2, 3\}$, can be exactly represented by a continuous superposition of evanescent plane waves, generalizing the standard Herglotz integral representation. Here, by evanescent plane wave, we mean an exponential plane wave $\mathbf{x} \mapsto e^{\imath\kappa \mathbf{d}\cdot\mathbf{x}}$, with complex-valued propagation vector $\mathbf{d} \in \mathbb{C}^n$. By construction, such a wave propagates along $\Re(\mathbf{d})$ and its absolute value decays exponentially along an orthogonal direction given by $\Im(\mathbf{d})$. A key result is that the density in the integral representation of the Helmholtz solution is proved to be uniformly bounded in a suitable weighted Lebesgue norm. We interpret this result as a stability property of evanescent plane waves, which is provably unattainable with only propagative plane waves. This paves the way for stable numerical computation of discrete expansions.

In view of practical implementations, discretization strategies of the integral representations are investigated. This essentially amounts to selecting appropriate direction vectors $\mathbf{d} \in \mathbb{C}^n$ for the waves in the approximation set. We propose a numerical recipe to construct suitable finite-dimensional sets of evanescent plane waves using simple sampling strategies in a parametric domain, following recent advances in approximation theory. Once the approximation sets are built, they can be used in a numerical scheme, such as a Trefftz Discontinuous Galerkin method for instance. Provided one uses sufficient oversampling and regularization techniques, numerical experiments show that the resulting approximations are both controllably accurate and numerically stable.

Geometry-based approximation of waves propagating through complex domains

Monica Nonino & Davide Pradovera & Ilaria Perugia *(University of Vienna)*

In this talk we will focus our attention on wave propagation problems in space and time. The spatial domain is assumed to be 2-dimensional, with piecewise-linear boundaries, and it can possibly include polygonal scatterers: we further assume that the wave cannot penetrate those scatterers.

We are interested in obtaining a numerical approximation of the solution of such problems, in the framework of model order reduction. With this goal in mind, I will present a surrogate model for the approximation of the propagating wave. In the model, the wave is approximated by the sum of some nonlinear functions. Each term in this sum represents a ray, which contributes to the approximation of the solution of the original problem, by modeling either a reflection or a diffraction effect. I will show how it is possible to identify these rays automatically, based only on the informations on the geometry of the domain. In particular, we will also discuss the possibility to control the number of terms to be used in the surrogate model in order to approximate the solution of the problem. Several numerical examples will showcase the potential of the proposed methodology.

At the end, I will draw some conclusions on the posi-

tive aspects of the proposed method, as well as some future perspectives and directions of research.

Keywords: wave propagation, model reduction, scattering, geometrical optics, diffraction

References

[1.] D.A. McNamara, C.W. Pistorius, J. Mahlerbe. *Introduction to the uniform geometrical theory of diffraction.* Artech House Norwood, 1990.

[2.] K. Greif, C. Urban. *Decay of the Kolmogorov N width for wave problems.* Applied Mathematics Letters, 96:216-222, 2019.

[3.] S.F. Potter, M.K. Cameron, R. Duraiswami. *Numerical geometric acoustics: an eikonal-based approach for modeling sound propagation in 3D environments.* arXiv, 2022.

[4.] D. Pradovera, M. Nonino, I. Perugia. *Geometry-based approximation of waves propagating through complex domains.* arXiv, 2023.

Scattering instabilities for metamaterial cavities

Camille Carvalho & Zoïs Moitier *(Univ Lyon, INSA Lyon, UJM, UCBL, ECL, CNRS UMR 5208, ICJ UC Merced)*

It is well-known that classical optical cavities can exhibit localized phenomena associated to scattering resonances, leading to numerical instabilities in approximating the solution [1]. For metamaterial cavities (optical cavities with negative optical properties) it is less clear whether similar phenomena arise. Additionally, localized bevahiors at the metamaterial-dielectric interface (such as the so-called surface plasmons) can emerge. In this talk we present how to establish the existence of metamaterial scattering resonances, and how they create numerical instabilities, this for arbitrary two-dimensional smooth metamaterial cavities (and varying optical parameter) [2]. The method relies on an asymptotic characterization of the resonances, and showing that problems with a sign-changing coefficient naturally fit the black box scattering framework via the "quasimodes to resonances" argument [3]. Numerical examples for several metamaterial cavities are provided.

References

[1.] S. Balac, M. Dauge, and Z. Moitier. Asymptotics for 2D whispering gallery modes in optical micro-disks with radially varying index. *IMA J. Appl. Math.*, 86(6):1212–1265, 2021. doi:10.1093/imamat/hxab033.

[2.] C. Carvalho, and Z. Moitier. Scattering resonances in unbounded transmission problems with sign-changing coefficient. *IMA J. Appl. Math.*, 0272-4960, 2023. 10.1093/imamat/hxad005.

[3.] S.-H. Tang and M. Zworski. From quasimodes to resonances. *Math. Res. Lett.*, 5(3):261–272, 1998. doi:10.4310/MRL.1998.v5.n3.a1.

This work is partially funded by the National Science Foundation Grant DMS-2009366.

Localized implicit time-stepping for the acoustic wave equation

Roland Maier & Dietmar Gallistl *(Friedrich Schiller University Jena)*

This talk is about locally computing solutions to the acoustic wave equation with possibly highly oscillatory coefficients. We rigorously prove that the localized (and especially parallel) computation on multiple overlapping subdomains is reasonable, making use of exponentially decaying entries of the global system matrices and an appropriate partition of unity. Moreover, a re-start is introduced after a certain amount of time steps to maintain a moderate overlap of the subdomains. Overall, the approach may be understood as a domain decomposition strategy (in space and time) that completely avoids inner iterations. Numerical experiments are presented that confirm the theoretical findings.

An $O(h)$ conforming VIE method for acoustic scattering by fractal inhomogeneities

Joshua Bannister, Andrew Gibbs, David P. Hewett & Valery Smyshlyaev (*University College London*)

The inhomogeneous Helmholtz equation

$$\Delta u + k^2 n u = 0, \quad \text{in } \mathbb{R}^2$$

where n is the refractive index, and the total field u is produced by an incident field u^{inc}, is a classical model for acoustic scattering by a compactly supported inhomogeneity $D = \text{supp}(1-n)$ and can be reformulated into the Lippmann-Schwinger equation [1, Chapter 9]

$$u(x) + k^2 \int_D (1 - n(y))\, G_k(|x-y|) u(y) dy = u^{inc}(x),$$

$x \in \mathbb{R}^2$. (1)

We are interested in numerical solutions of (1) when n takes a constant value on a self-similar volume D with a fractal boundary, such as the Koch snowflake. A naïve method is to approximate D with a sequence of smoother (e.g. Lipschitz) "pre-fractals" $\{D_j\}_{j=1}^{\infty}$, apply a piecewise constant Galerkin FEM method on each D_j, with mesh-width h_j, and study the joint limit as $h_j \to 0$ and $j \to \infty$. Although this method converges, misapproximating the fractal boundary ∂D leads to a "fractal stair-casing" error, giving the method a rate of convergence of $O(h_j^{1-d/2})$, where d denotes the Hausdorff dimension of ∂D.
In this talk, we present a novel discretisation method which exploits the self-similarity of D to eliminate this stair-casing error by meshing the self-similar set D with scaled copies of itself. This allows us to define piecewise constant approximation spaces on these self-similar meshes and show that the associated Galerkin approximations are quasi-optimal, stable and converge linearly with mesh width. Using recent fractal quadrature rules [2, 3], we exploit the self-similarity of the mesh and properties of the fundamental solution $G_k(\cdot,\cdot)$ to compute the entries of the resulting Galerkin matrix with quadratic accuracy in the quadrature size parameter, for both regular and singular interactions. We then adapt Strang's first lemma to this context and provide a fully discrete error analysis. Finally, we exploit the geometry of the mesh to accelerate iterative solutions of the resulting dense linear system via an FFT-based circulant-embedding method, resulting in $O(N)$ storage of the linear system and $O(N \log N)$ operations per iteration, where N denotes the number of self-similar elements in the mesh.

References

[1.] D. Colton and R. Kress, *Inverse acoustic and electromagnetic scattering theory*, vol. 93 of Applied Mathematical Sciences, Springer, Cham., 2019. Fourth edition.

[2.] A. Gibbs, D. Hewett and A. Moiola, *Numerical quadrature for singular integrals on fractals*, Numer. Algorithms, 92 (2023), pp. 2071–2124.

[3.] A. Gibbs, D.P. Hewett and B. Major, *Numerical evaluation of singular integrals on non-disjoint self-similar fractal sets*, arXiv preprint arXiv:2303.13141, (2023).

Minisymposium M4

Recent advances in the approximation of variational inequalities

Organisers
Mira Schedensack and Philip Lederer

Two Discretisations of the Time-Dependent Bingham Problem

Mira Schedensack & Carsten Carstensen *(Universität Leipzig)*

This talk introduces a non-conforming Crouzeix-Raviart approximation of the stationary three-dimensional Bingham problem and the two-dimensional Mosolov problem for the flow in a pipe. The non-conformity allows for quasi optimal error estimates in contrast to the standard conforming $P1$ finite element scheme. Moreover, this space discretisation is combined with two time-discretisations for the corresponding time-dependent problems. The first time discretisation is a generalised midpoint rule and the second time discretisation is a discontinuous Galerkin scheme. The a priori error analyses for both schemes yield certain convergence rates in time and optimal convergence rates in space. It guarantees convergence of the fully-discrete scheme with a discontinuous Galerkin time-discretisation for consistent initial conditions and a source term $f \in H^1(0,T;L^2(\Omega))$.

dG for elastoplastic evolution?

Carsten Carstensen *(Humboldt-Universität zu Berlin)*

The discontinuous Galerkin (dG) methodology provides a hierarchy of time discretization schemes for evolutionary problems such as elastoplasticity with the Prandtl-Reuß flow rule. A first dG time discretization has been proposed for a variational inequality modeling rate-independent inelastic material behaviour in Alberty and Carstensen in (CMME 191:4949-4968, 2002) with the help of duality in convex analysis to justify certain jump terms. The presentation shall discuss the scheme and the error estimates from recent paper of Carstensen, Liu, and Alberty in (Numer. Math. 141: 715-742, 2019) based on a seemingly sharp error analysis. The numerical investigation for

a benchmark problem with known analytic solution provides empirical evidence of a higher convergence rate of the dG(1) scheme compared to dG(0).

Error analysis for a distributed optimal control problem governed by the von Kármán equation

Asha K. Dond & Sudipto Chowdhury, Devika Shylaja, Neela Nataraj *(Indian Institute of Science Education and Research)*

The numerical analysis of the distributed optimal control problem governed by the von Kármán equation specified on a polygonal domain in R^2 will be discussed in this talk. The nonconforming Morley finite element method is used to discretize the state and adjoint variables, while piecewise constant functions are used to discretize the control. For the state, adjoint, and control variables, a priori and a posteriori error estimates are derived. A posteriori error estimates are also shown to be efficient. Finally, we'll see some numerical results that confirm the theoretical estimates.

A posteriori analysis for Bingham via equilibrated fluxes

Alexei Gazca *(University of Freiburg)*

The accurate simulation of viscoplastic fluids can be extremely challenging due to the non-smoothness of the constitutive relations that describe them. Methods that do not regularise the constitutive relation and solve directly the underlying variational inequality are preferred by practitioners, since they tend to result in more accurate simulations; popular non-smooth methods are those based on augmented Lagrangians (ALG2/ ADMM) and proximal gradients (FISTA*). One of the drawbacks of such methods is that they can be slow to converge; to alleviate this, subproblems at each iteration are often solved inexactly, based on heuristic stopping criteria. In this work we derive a posteriori estimates within the framework of equilibrated fluxes for non-smooth formulations of Bingham flow; we prove a guaranteed upper bound and local efficiency of a posteriori estimators that distinguish the various components of the error. This allows us to develop inexact adaptive versions of ALG2/FISTA*, that are able to balance the errors caused by discretisation, linearisation and algebraic solvers.

Mass Conserving Mixed Stress-Strain rate Finite Element Method for Non-Newtonian Fluid Simulations

Jan Ellmenreich[1] and Philip L. Lederer[2 1] *(TU Wien)* [2] *(University of Twente)*

Many non-Newtonian models assume a non-linear relation between the deviatoric stress tensor $\boldsymbol{\tau}$ and the rate-of-strain tensor $\boldsymbol{\varepsilon}(\boldsymbol{u})$, which is not necessarily given in explicit form. Therefore a crucial requirement on a finite element method is the capability to capture the behaviour of the non-linear constitutive relation.

Assuming incompressible, stationary, isothermal, laminar flow, we extend the finite element method proposed in [1] by additionally approximating the rate-of-strain tensor $\boldsymbol{\varepsilon}(\boldsymbol{u})$. The introduction of such a variable allows a natural embedding of a general implicit constitutive relation of the form $G(\boldsymbol{\tau}, \boldsymbol{\varepsilon}(\boldsymbol{u})) := 0$, and $H(\mathrm{div})$-conforming velocity approximations result in exact conservation of mass.

We discuss the solvability of the novel formulation and present several numerical examples with various constitutive laws.

References

[1.] Jay Gopalakrishnan, Philip L. Lederer, and Joachim Schöberl. *A mass conserving mixed stress formulation for Stokes flow with weakly imposed stress symmetry.* IMA Journal of Numerical Analysis, Vol. 40, Iss. 3, pp. 1838-1874, 2020.

Mixed finite elements for Bingham flow in a pipe

Philip L. Lederer & Tom Gustafsson *(University of Twente)*

We consider mixed finite element approximations of viscous, plastic Bingham flow in a cylindrical pipe. A novel a priori and a posteriori error analysis is introduced which is based on a discrete mesh dependent norm for the normalized Lagrange multiplier. This allows proving stability for various conforming finite elements. Numerical examples are presented to support the theory and to demonstrate adaptive mesh refinement.

A posteriori error estimates for variational inequalities discretized by higher-order finite elements

Andreas Schröder & Lothar Banz *(Paris Lodron University Salzburg)*

The talk presents a posteriori error estimates for variational inequalities with linear constraints. The error estimates are derived using an abstract framework in which the error contributions representing non-penetration, non-conformity and complementarity conditions form a weighted functional. The use of the minimizer of this functional enables the derivation of reliable and efficient a posteriori error estimates. The abstract findings are applied, in particular, to the obstacle problem and to the simplified Signorini problem, where higher-order finite elements are used for discretization. Several numerical experiments are presented to discuss the properties of the error estimates and their applicability in adaptive schemes.

Minisymposium M5

Saddle point problems: solvers and preconditioners

Organisers

Erin Carson and Ieva Daužickaité

Adaptive coarse spaces for saddle point problems

Frédéric Nataf & Pierre-Henri Tournier *(Sorbonne Université)*

We introduce a scalable adaptive element-based domain decomposition (DD) method for solving saddle point problems defined as a block two by two matrix. Such linear systems are ubiquitous in scientific computing. The stable discretization of equations for (nearly) incompressible fluids or elastic bodies requires a velocity-pressure formulation. Our algorithm does not require any knowledge of the constrained space. We assume that all sub matrices are sparse and that the diagonal blocks are spectrally equivalent to a sum of positive semi definite matrices. The latter assumption enables the design of adaptive coarse space for DD methods that extends the GenEO theory to saddle point problems. Numerical results on three- dimensional elasticity problems for steel-rubber structures discretized by a finite element with continuous pressure are shown for up to one billion degrees of freedom along with comparisons to Algebraic Multigrid Methods and direct solvers. The method has also been applied to Stokes system with discontinuous coefficients.

Preconditioned Iterative Solvers for Instationary Fluid Flow Control Problems

John Pearson *(University of Edinburgh)* & Santolo Leveque *(Scuola Normale Superiore, Pisa)*

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 some function arising from a particular physical objective, while at the same time obeying a system of PDEs which describe the process. It is necessary to obtain accurate solutions to such problems within a reasonable CPU time, in particular for time-dependent problems, for which the "all-at-once" solution can lead to extremely large linear(ized) systems.

In this talk we consider iterative methods, in particular Krylov subspace methods, to solve fluid flow control problems where the Stokes or Navier–Stokes equations form the PDE constraints. Whereas the methodology described in this talk can also be applied to stationary problems, we focus on the instationary case here. We employ a Picard (or Oseen-type) outer iteration for Navier–Stokes problems, and derive fast and robust preconditioners for the flexible GMRES method when solving the large-scale systems of equations that result. We employ an inner solver to the leading block of these systems, for which we may apply existing preconditioners for heat and convection–diffusion control problems. To approximate the Schur complement, we devise a block-version of a commutator argument used for matrices that involve products of divergence and gradient terms. Numerical results demonstrate the effectiveness of the preconditioning approach.

Saddle Point Preconditioners for Weak-Constraint Four-Dimensional Variational Data Assimilation

Jemima M. Tabeart & John W. Pearson *(University of Oxford)*

Data assimilation algorithms blend observation data together with prior information from a numerical model to obtain an improved estimate of the current state of a dynamical system of interest. In this setting, the

use of correlated observation error covariance matrices has produced many opportunities for improved initial conditions for weather forecasts, but at the risk of more ill-conditioned linear systems which can be prohibitively expensive to solve. In this talk I will present novel preconditioners for a saddle point formulation of the weak-constraint 4DVar data assimilation problem, with a focus on the correlated observation error setting.

I will present a number of new preconditioners that improve on current state-of-the-art, and allow for reductions in computational cost through the use of parallel architectures or matrix-oriented iterative methods.

Fast numerical solvers for pattern formation problems in mathematical biology

Karolína Benková & John Pearson & Mariya Ptashnyk *(MAC-MIGS, Heriot-Watt University & University of Edinburgh)*

Many of the mechanisms governing pattern formation in embryonic development have been identified and described by systems of PDEs. As some of the parameters or functions in these PDEs may be impossible to measure in laboratory conditions, we can use optimal control theory, in particular PDE-constrained optimization, to identify them. Given experimental data as the desired states, we can pose a minimisation problem so that the equations in the constraints evolve the state as close as possible to the desired state while also minimising the amount of control (or external biological mechanism) applied. In this talk, we will present a numerical solver for a problem with reaction-diffusion PDEs as constraints, by making use of a preconditioner for the large-scale saddle-point problems that arise.

Some preconditioning techniques for a class of double saddle point linear systems

Luca Bergamaschi *(University of Padua)*

In this contribution, we describe and analyze the spectral properties of a number of block preconditioners for a class of double saddle point problems [1, 3]. We focus our attention to an inexact version of a block triangular preconditioner providing extremely fast convergence of the FGMRES method. We develop a spectral analysis of the preconditioned matrix showing that the complex eigenvalues lie in a circle of center $(1, 0)$ and radius 1, while the real eigenvalues are described in terms of the roots of a third order polynomial with real coefficients [2]. Numerical examples are reported to illustrate the efficiency of inexact versions of the proposed preconditioners, and to verify the theoretical bounds. The proposed preconditioners will be tried onto real-life test problems arising in coupled poromechanics [4].

In collaboration with F. Bakrani Barani, M. Hajarian, Department of Applied Mathematics, Faculty of Mathematical Sciences, Shahid Beheshti University, Tehran, Iran, and A. Martínez, Department of Geosciences, University of Trieste, Italy

References

[1.] F. Bakrani Balani, L. Bergamaschi, M. Hajarian, Two block preconditioners for a class of double saddle point linear systems, *Applied Numerical Mathematics*, 2023, to appear.

[2.] F. Bakrani Balani, L. Bergamaschi, A Martínez, M. Hajarian, Some preconditioning techniques for a class of double saddle point problems. *in preparation*, 2023.

[3.] S. Bradley, C. Greif, Eigenvalue bounds for double saddle-point systems, *arXiv:2110.13328* [math.NA], 2021.

[4.] M. Frigo, N. Castelletto, M. Ferronato, and J. White, Efficient solvers for hybridized three-field mixed finite element coupled poromechanics, *Comput. Math. Appl.*, 91 (2021), pp. 36–52.

Randomized preconditioning for least squares iterative refinement

Ieva Daužickaité & Erin Carson *(Charles University)*

Employing low precision in algorithms for solving various computational problems can improve the performance, but it comes at a price of reduced accuracy. Mixed precision algorithms aim to exploit the benefits of low precision while also obtaining a high accuracy solution. One such method is iterative refinement (IR) for least squares problems, that requires solving a series of saddle point systems of linear equations with changing right hand sides. Solving these via GMRES preconditioned with QR factors of the least squares coefficient matrix A allows tackling highly ill conditioned problems. However computing QR decomposition of

a large A can be expensive. Preconditioners based on the QR factorisation of a randomly sketched A have been shown to be effective for dense least squares problems solved via LSQR. In this talk, we explore how such preconditioners can be used in the least squares IR setting.

Minisymposium M6

Numerical methods for fractional-derivative problems
Organisers
Natalia Kopteva and Yubin Yan

Discovering the subdiffusion model in an unknown medium

Zhi Zhou & Siyu Cen, Bangti Jin, Yikan Liu *(Hong Kong Polytechnic University)*

The subdiffusion phenomenon is now widely recognized in many engineering and physical applications. The mathematical models for subdiffusion involve many parameters, e.g., diffusion coefficient, potential, initial and boundary conditions, source along with the order of derivation. Sometimes some of these parameters are not readily available, but one can measure additional information about the solution. Then one natural question is how much we can say about the mathematical model. In this talk, I will discuss several theoretical and computational results on determining the several parameters from one measurement when the other problem data are not fully specified.

Galerkin finite element approximation of a stochastic semilinear fractional subdiffusion with fractionally integrated additive noise

Yubin Yan *(University of Chester)*

A Galerkin finite element method is applied to approximate the solution of a semilinear stochastic space and time fractional subdiffusion problem with the Caputo fractional derivative of the order $\alpha \in (0,1)$, driven by fractionally integrated additive noise. After discussing the existence, uniqueness and regularity results, we approximate the noise with the piecewise constant function in time in order to obtain a regularized stochastic fractional subdiffusion problem. The regularized problem is then approximated by using the finite element method in the spatial direction. The mean squared errors are proved based on the sharp estimates of the various Mittag-Leffler functions involved in the integrals. Numerical experiments are conducted to show that the numerical results are consistent with the theoretical findings.

This is a joint work with Prof. Amiya Pani, IIT Bombay, India.

Detailed Error Analysis for a Fractional Adams Method on Caputo—Hadamard Fractional Differential Equations

Charles W.H. Green & Yubin Yan *(University of Chester)*

In this work, we considered a predictor–corrector numerical method for solving a Caputo–Hadamard fractional differential equation over the uniform mesh $\log t_j = \log a + \left(\log \frac{t_N}{a}\right)\left(\frac{j}{N}\right)$, $j = 0, 1, 2, \ldots, N$ with $a \geq 1$, where $\log a = \log t_0 < \log t_1 < \cdots < \log t_N = \log T$ is a partition of $[\log a, \log T]$. We consider the error estimates under the different smoothness properties of the solution y and the nonlinear function f. Numerical examples are given to verify that the numerical results are consistent with the theoretical results.

A comparison of some numerical methods for shifted fractional Laplacians

Lehel Banjai *(Heriot-Watt University)*

In the last couple of decades there has been an explosion of interest in fractional differential equations, and in particular in models involving a fractional power of the Laplacian in the context of anomalous diffusion. Concurrently a large number of numerical methods have been developed and analysed. Many of the latter (though not all) can be understood as rational approximations of the fractional power or its inverse. This is the case for classes of contour integral methods and their quadratures as well as tensor product discretisations of extensions to degenerate (but local) elliptic problems. We consider these methods applied to shifted fractional Laplacian problems of the form

$$(-\Delta)^s u - k^{2s} u = f, \qquad s \in (0,1),$$
$$k^2 \in \{\mathbb{C} \setminus (-\infty, 0]\} \cup \sigma(-\Delta),$$

where $-\Delta$ is the Dirichlet Laplacian. Such problems are either of independent interest, or arise as a result of time-stepping. We will give a new representation

of the solution operators of the above problem for a particular class of shifts and compare theoretically and numerically some of the different approaches.

Convergence of numerical methods for fractional diffusion equations with boundaries

Ercília Sousa (University of Coimbra)

We consider a model that consists on the fractional diffusion equation with Dirichlet boundary conditions and discretize it with an implicit numerical method. The discretization chosen for the spatial fractional differential operator is known to be second-order accurate, when the problem is defined in the real line. We show that the order of accuracy of the spatial truncation error can be lower than two in the presence of the boundary and in some cases we have inconsistency. Furthermore, we prove the rate of convergence will be higher than the order of accuracy given by the consistency analysis and sometimes we can recover the order two.

Exponential convergence of *hp*-FEM for the integral fractional Laplacian

Markus Faustmann *(TU Wien)* & Carlo Marcati *(University of Pavia)* & Jens Markus Melenk *(TU Wien)* & Christoph Schwab *(ETH Zürich)*

In this talk, we consider PDEs involving fractional powers of the Laplacian $(-\Delta)^s$ for $s \in (0,1)$, using the singular integral definition. Solutions to fractional PDEs are known to lose regularity near the whole boundary of the computational domain.

On polygonal domains (2D) or polyhedral domains (3D), we establish a precise description of the regularity of solutions for analytic data in suitably weighted Sobolev spaces reflecting both the analytic nature inside the domain and the anisotropic singular behaviour near the boundary. Unlike local elliptic operators in polygons, fractional operators in polygons require not only vertex-weighted but also additionally edge-weighted spaces.

Weighted analytic regularity results of our type are then used to design exponentially convergent *hp*-finite element approximations on suitable anisotropic geometric meshes.

References

[1.] J.P. Borthagaray, R.H. Nochetto. *Besov regularity for the Dirichlet integral fractional Laplacian in Lipschitz domains*, J. Funct. Anal. 284 (2023), no. 6, Paper No. 109829.

[2.] M. Faustmann, C. Marcati, J.M. Melenk, Schwab, Ch. *Weighted analytic regularity for the integral fractional Laplacian in polygons*, SIAM J. Math. Anal., 54 (2022), 6323-6357.

[3.] M. Faustmann, C. Marcati, J.M. Melenk, Schwab, Ch. *Exponential Convergence of hp FEM for the Integral Fractional Laplacian in Polygons*, arXiv:2209.11468 (2022).

Pointwise-in-time a-posteriori error control for time-fractional parabolic equations

Natalia Kopteva *(University of Limerick)*

For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0,1)$, we give pointwise-in-time a posteriori error bounds in the spatial L_2 and L_∞ norms. Hence, an adaptive time stepping algorithm is applied for the L1 method, which yields optimal convergence rates $2-\alpha$ in the presence of solution singularities. Interestingly, the proposed time stepping algorithm yields the grids similar to a-priori-constructed optimal grids in [2, 3].

We shall also briefly discuss an extension of the proposed methodology to variable-coefficient multiterm time-fractional subdiffusion equations [4], while the case of higher-order discretizations [5] will be discussed in the accompanying talk by Sebastian Franz.

References

[1.] N. Kopteva, *Pointwise-in-time a posteriori error control for time-fractional parabolic equations*, Appl. Math. Lett., 123 (2022), 107515.

[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 for time-fractional semilinear parabolic equations using upper and lower solutions*, SIAM J. Numer. Anal., 58 (2020), 2212–2234.

[4.] N. Kopteva and M. Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, J. Sci. Comput., (2022).

[5.] S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, J. Comput. Appl. Math., volume 427 (2023), 115122.

Efficient and stable implementation of higher order methods for time-dependent fractional parabolic equations

Sebastian Franz & Natalia Kopteva *(TU Dresden)*

In this talk we consider the fractional-order parabolic equation

$$D_t^\alpha u + Lu = f(x,t) \qquad \text{for } (x,t) \in \Omega \times (0,T]$$

with an initial condition $u(\cdot,0) = u_0$ in Ω and the boundary condition $u = 0$ on $\partial\Omega$ for $t > 0$, where $\alpha \in (0,1)$ and L is a spatial second-order elliptic operator. The fractional derivative is the Caputo fractional derivative in time, defined for $t > 0$ by

$$\begin{aligned} D_t^\alpha u &:= J_t^{1-\alpha}(\partial_t u), \qquad J_t^{1-\alpha} v(\cdot,t) \\ &:= \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, v(\cdot,s)\, ds, \end{aligned}$$

where $\Gamma(\cdot)$ is the Gamma function, and ∂_t denotes the partial derivative in t.

The fractional operator is by nature a non-local operator, which poses a major problem in the implementation of numerical methods for solving the equation. Typically, round-off errors and numerical instabilities cause the errors to grow so that the computed solutions can be far from the exact ones. This is especially true for higher order methods, which are more affected by these error sources.

We apply rewriting and adaptive quadrature techniques in order to obtain stable implementations for several different methods, starting with the classical L1-method and also for its generalisations in the form of collocation methods. We use the adaptive mesh-generation algorithm presented by Natalia Kopteva in a separate talk, which has the advantage of being able to deal with initial singularities and local irregularities in the solution. We present numerical simulations confirming stability and good convergence behaviour. Our results are reliable for α in the range of at least 0.1 and 0.999, and for meshes with mesh sizes that support a global error of 10^{-8} measured in the L^∞-norm.

References

[1.] S. Franz and N. Kopteva. Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations. *J. Comp. Appl. Math.*, 2023. accepted, arXiv:2211.06272.

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, 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. We propose an extension to the approach, by Kopteva and Meng [1], used to analyse the error of L1-type discretizations on both graded and uniform temporal meshes. We broaden the assumption on the regularity of the solution to incorporate more general solution behaviour, such that $|\delta_t^l u(\cdot,t)| \lesssim 1 + t^{\sigma-l}$ for $\sigma \in (0,1) \cup (1,2)$ and $l = 0,1,2$. 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 in [2]). Extensions to the semilinear case will also be considered.

References

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

[2.] Dongfang Li, Hongyu Qin, and Jiwei Zhang. *Sharp pointwise-in-time error estimate of L1 scheme for nonlinear subdiffusion equations*, https://doi.org/10.48550/arXiv.2101.04554, (2021).

Minisymposium M7

Recent Advances in finite element methods

Organisers

Mark Ainsworth and Charles Parker

Recent Developments in High Order Finite Element Approximation

Mark Ainsworth *(Brown University)* & Charles Parker *(University of Oxford)*

We give a brief overview of our recent work on high order finite element approximation ranging from pressure robust methods for incompressible flow that are uniformly stable in both the mesh size and the polynomial degree to preconditioners that are also uniform in the mesh size and the polynomial degree.

A uniformly *hp*-stable element for the stress complex

Francis Aznaran, Kaibo Hu, & Charles Parker *(University of Oxford)*

For the Hellinger–Reissner principle of stress-displacement linear elasticity, we prove inf-sup stability bounds which are independent of polynomial degree and mesh size, for a novel sequence of conforming finite element spaces discretising the stress elasticity complex in two dimensions. The stress space coincides with the symmetry-enforcing Hu–Zhang element, of which we provide a novel characterization. This may be achieved via the construction of a bounded right inverse of the divergence operator, on the discontinuous Lagrange element which discretises the displacement, by adapting techniques used to proved the analogous statement for the Falk–Neilan pair for incompressible Stokes flow.

Our main novelty, however, lies in an alternative proof via the construction of bounded Poincaré operators for the elasticity complex which are polynomial-preserving, in the Bernstein–Gelfand–Gelfand framework of the finite element exterior calculus. Numerical examples are provided.

Multigrid solvers for the de Rham complex with optimal complexity in polynomial degree

Pablo D. Brubeck & Patrick E. Farrell *(University of Oxford)*

The Riesz maps of the L^2 de Rham complex frequently arise as subproblems in the construction of fast preconditioners for more complicated problems. In this work we present multigrid solvers for high-order finite element discretizations of these Riesz maps with the same time and space complexity as sum-factorized operator application, i.e., with optimal complexity in polynomial degree in the context of Krylov methods. The key idea of our approach is to build new finite elements for each space in the de Rham complex with orthogonality properties in both the L^2- and $H(\mathrm{d})$-inner products ($\mathrm{d} \in \{\mathrm{grad}, \mathrm{curl}, \mathrm{div}\}$) on the reference hexahedron. The resulting sparsity enables the fast solution of the patch problems arising in the Pavarino, Arnold–Falk–Winther, and Hiptmair space decompositions, in the separable case. In the non-separable case, the method can be applied to an auxiliary operator that is sparse by construction. With exact Cholesky factorizations of the sparse patch problems, the application complexity is optimal but the setup costs and storage are not. We overcome this with the finer Hiptmair space decomposition and the use of incomplete Cholesky factorizations imposing the sparsity pattern arising from static condensation, which applies whether static condensation is used for the solver or not. This yields multigrid relaxations with time and space complexity that are both optimal in the polynomial degree.

We illustrate our preconditioning approach by solving mixed formulations of the Hodge–Laplacian and the vorticity-velocity-pressure formulation of Stokes flow, for which we observe robustness with respect to the mesh size and the polynomial degree.

Tensor product finite element BGG complexes

Kaibo Hu & Francesca Bonizzoni & Guido Kanschat & Duygu Sap *(University of Oxford)*

We construct discrete versions of Bernstein-Gelfand-Gelfand (BGG) sequences in any space dimension. Examples in 3D include the elasticity, the Hessian, and the divdiv complexes. The resulting spaces and complexes are tensor products of 1D complexes with various kinds of regularity. The tensor product structure also leads to bounded commuting quasi-interpolations.

Implementing high order C^1-conforming elements with C^0 elements

Charles Parker *(University of Oxford)* & Mark Ainsworth

High order numerical methods are known to provide exponential rates of convergence for problems containing singularities and boundary layers. Such features are typical in engineering problems including plates and shells. However, conforming approximation of such problems often requires C^1 continuity which, unfortunately, rules out the use of many, if not all, existing finite element codes. We describe the details needed for the efficient implementation of arbitrar-

ily high order finite elements with C^1 continuity using only standard C^0 and discontinuous finite element spaces. The method is illustrated by applying it to the solution of a number of representative test problems.

Minisymposium M8

Spectral methods and orthogonal polynomials
Organisers
Timon Gutleb, Ioannis Papadopoulos and Marco Fasondini

Numerical analytic continuation

Lloyd N. Trefethen *(University of Oxford)*

Spectral methods for PDEs start from the idea of exploiting analyticity of solutions, which quickly leads to the questions, how and how far can a solution be analytically continued across the boundary? Numerical analytic continuation is impossible or at least highly ill-conditioned in theory, depending how you frame the problem, yet sometimes surprisingly tractable in practice. The outline of the talk will be as follows:
(1) Theorems (pretty gloomy)
(2) Blending functions and "fat branch cuts"
(3) Experiments (pretty encouraging)
(4) The one-wavelength principle
(5) The Schwarz function

Convergence and Near-optimal Sampling for Multivariate Function Approximations in Irregular Domains via Vandermonde with Arnoldi

Wenqi Zhu & Yuji Nakatsukasa *(University of Oxford)*

Vandermonde matrices are usually exponentially ill-conditioned and often result in unstable approximations. In this talk, we would like to introduce and discuss the *multivariate Vandermonde with Arnoldi (V+A) method*, which is based on least-squares approximation together with a Stieltjes orthogonalization process, for approximating continuous, multivariate functions on d-dimensional irregular domains. The V+A method addresses the ill-conditioning of the Vandermonde approximation by creating a set of *discrete orthogonal basis* with respect to a discrete measure. The V+A method is simple and general. It relies only on the sample points from the domain and requires no prior knowledge of the domain. In the talk, we will analyze the sample complexity of the V+A approximation. In particular, we show that, for a large class of domains, the V+A method gives a well-conditioned and near-optimal N-dimensional least-squares approximation using $M = \mathcal{O}(N^2)$ equispaced sample points or $M = \mathcal{O}(N^2 \log N)$ random sample points, independently of d. We also give a comprehensive analysis of the error estimates and rate of convergence of the V+A approximation. Based on the multivariate V+A approximation, we propose a new variant of the weighted V+A least-squares algorithm that uses only $M = \mathcal{O}(N \log N)$ sample points to give a near-optimal approximation. Our numerical results confirm that the (weighted) V+A method gives a more accurate approximation than the standard orthogonalization method for high-degree approximation using the Vandermonde matrix.

Keywords: least-squares, Vandermonde matrix, Arnoldi, polyval, polyfit, ill-conditioning, sample complexity, near-optimal sampling

Avoiding discretization issues for nonlinear eigenvalue problems

Matthew J. Colbrook *(University of Cambridge)* & Alex Townsend *(Cornell University)*

The first step when solving an infinite-dimensional eigenvalue problem is often to discretize it. We show that one must be extremely careful when discretizing nonlinear eigenvalue problems. Using examples, we show that discretization can: (1) introduce spurious eigenvalues, (2) entirely miss spectra, and (3) bring in severe ill-conditioning. While there are many eigensolvers for solving matrix nonlinear eigenvalue problems, we propose a solver for general holomorphic infinite-dimensional nonlinear eigenvalue problems that avoids discretization issues, which we prove is stable and converges. Moreover, we provide an algorithm that computes the problem's pseudospectra with explicit error control, allowing verification of computed spectra. The algorithm and numerical examples are publicly available in `infNEP`, which is a software package written in MATLAB.

Computing Orthogonal Polynomials via Cholesky, QR and QL

Sheehan Olver *(Imperial College)*, Timon Gutleb *(University of Oxford)* & Mikael Slevinsky *(University of Manitoba)*

Orthogonal polynomials are traditionally computed using Gram–Schmidt/Lanczos. A classic result that is under-utilised is that they can be computed more stably using the Cholesky decomposition. When the weight is a polynomial modification of a known weight this reduces to Cholesky of an (infinite) banded matrix which can be computed in optimal complexity. This can be extended to rational modifications using *reverse Cholesky* (Cholesky from the bottom right), QR, and QL decompositions. This gives an effective tool for constructing families of semiclassical orthogonal polynomials, useful for sparse spectral methods on non-standard geometries such as disk slices, spherical caps, and annuli.

A spectral method for fractional integral equations using orthogonal fractional polynomials

Tianyi Pu & Marco Fasondini *(Imperial College London)*

We present a spectral method that achieves exponential convergence for a variety of one-sided linear fractional integral equations on a closed interval, including ones with single irrational order, multiple rational orders, non-trivial variable coefficients, and initial-boundary conditions. The method uses a basis consisting of orthogonal fractional polynomials that are obtained from an appropriate change of variable in classical Jacobi polynomials. We present algorithms for building the fractional integral operators, which are applied to the presented basis as infinite matrices. Generating the operators requires high-precision computing due to the instablity of existing algorithms, but the resulting linear systems are well-conditioned and the method is stable and efficient. For a problem arising from time-fractional heat and wave equations, we show that our method (which is not sparse but uses an orthogonal basis) outperforms a sparse spectral method (which uses a basis that is not orthogonal) due to its superior stability.

Spatial isometries in multivariate orthogonal polynomials

Richard Mikaël Slevinsky *(University of Manitoba)* & Jared Aurentz *(Universidad de Huelva)*

Univariate orthogonal polynomials are unique up to a normalization and a phase. Common normalizations include point evaluation and orthonormality, but the choice of phase (in particular real phase) is usually uninteresting. In the multivariate setting, the story of the phase could not be more different. In general, the dimension of the space of total degree-n mutually orthogonal polynomials is greater than one; thus, the multivariate analogue of a real (complex) phase is an orthogonal (unitary) matrix of connection coefficients between one family and another. Koornwinder produced a construction of multivariate orthogonal polynomials out of hierarchies of univariate classical orthogonal polynomials that are structurally akin to spherical harmonics. On the disk, two examples of this construction are the Zernike polynomials and the Dunkl-Xu polynomials. Moreover, three distinct families of Proriol polynomials live on the triangle. We explore sparse normal eigenvalue problems whose eigenvectors are the connection coefficients between two multivariate orthogonal polynomial families. On the disk, this enables the rotation of Dunkl-Xu polynomials, and spherical harmonics may also be rotated in this way. The code is freely available at https://github.com/MikaelSlevinsky/FastTransforms.

Sobolev-Orthogonal Bases from Standard-Orthogonal Polynomials

Marcus Webb *(University of Manchester)*

The Fourier transform of an orthogonal polynomial basis multiplied by an appropriate fixed function yields a basis of functions with a tridiagonal, skew-Hermitian differentiation matrix. Given any orthogonal polynomial basis, a cascade of associated bases can be constructed which are orthogonal with respect to Sobolev inner products. Each basis in the cascade is associated with a rational modification of the weight function of the original orthogonal polynomial basis. The connection coefficients between each basis in the cascade are banded triangular matrices, a consequence of which is that properties such as the existence of fast transforms and spectral approximation properties are a feature of all or none of the bases in the cascade. We will conclude the talk by showing how to generate bases that are orthogonal with respect to more exotic, weighted Sobolev inner products, via the Lanczos or Arnoldi iterations applied to the differential operator. This is joint work with Arieh Iserles (University of Cambridge).

Solving nonlinear ODEs with the ultraspherical spectral method

Kuan Xu & Ouyuan Qin *(University of Science and Technology of China)*

We extend the ultraspherical spectral method to solving nonlinear ODE boundary value problems. We propose to use the inexact Newton-GMRES framework for which an effective preconditioner can be constructed and a fast Jacobian-vector multiplication can be effected, thanks to the structured operators of the ultraspherical spectral method. With a mixed-precision implementation, the inexact Newton-GMRES-ultraspherical framework exhibits extraordinary speed and accuracy, as we show by extensive numerical experiments.

Sparse spectral methods for fractional PDEs

Ioannis P. A. Papadopoulos & Sheehan Olver *(Imperial College London)*

Fractional partial differential equations (FPDEs) model nonlocal processes such as sound wave absorption in the brain, long-range geophysical effects, and Lévy flights. Many methods require a truncation of the domain to discretize. Aside from the expense, the nonlocal nature of FPDEs and the slow decay of the solutions often cause numerical artefacts to appear even with large truncations. Moreover, the solutions may exhibit singularities that must be accounted for to build methods that converge quickly.

We discuss a class of FPDEs that include fractional Laplacian, derivative, Hilbert transform, and identity operators. By constructing a sum space consisting of weighted Chebyshev polynomials of the second kind and their Hilbert transform counterparts, we precisely identify the action of the fractional operator on our approximation space. This allows us to derive sparse relationships between the sum space that we expand our solution in, and the right-hand side which is expanded in the so-called dual sum space. Affine transformations of the sum space may be combined in the approximation where, remarkably, the action of the fractional operator decouples. Hence, we solve over each interval separately and in parallel.

We apply our spectral method to problems with smooth data, where we observe spectral convergence, as well as fractional heat and wave propagation problems.

Sphere we go again: polynomials in polar coordinates

Geoff Vasil *(University of Edinburgh)*

This talk will present some recent progress on systems of polynomials for computations in multi-dimensional spheres and balls. Spherical harmonics and Zernike polynomials form the foundation for this classical field. However, the talk will discuss more recent improved understanding of a generalised framework, unifying computations in both spheres and disks into a differential/algebraic calculus based on continuous/discrete orthogonal polynomials. Moreover, the scheme includes both tensorial and scalar-valued functions and also ascribes new meaning to simple edge cases resulting from ordinary circles and intervals.

Spectral Methods for the Debye-Smoluchowski Equation

Georgia Bradshaw *(University of Manchester)*

The Debye-Smoluchowski equation describes the change in dynamics in Inhomogeneous Chemical Kinetics systems due to the effects of charged chemical species' interacting with each other. Solving this equation includes the calculation of the induced electric field via an integral of the charge distribution, and the divergence of a given field, both of which can be calculated quickly and accurately using Spectral Methods.

Here, focusing on the trigonometric basis ($\sin(\omega_n x)$ or $\cos(\omega_n x)$), we show that the change in dynamics due to charge effects can be calculated efficiently by taking advantage of ready-made algorithms for discrete sine and cosine transforms.

A static memory sparse spectral method for time-fractional PDEs

Timon S. Gutleb & José A. Carrillo *(University of Oxford)*

Fractional differential equations generalize ODEs and PDEs to include derivative operators of non-integer order – the resulting operators are generally nonlocal and pose several challenges to conventional numerical approaches. In my talk I will present a method which provides accurate numerical solutions to fractional-in-time partial differential equations without the excessive memory requirements usually associated with the nonlocal fractional derivative operator. Our approach combines recent advances in the development and utilization of multivariate sparse spectral methods as well as fast methods for the computation of Gauss quadrature nodes with recursive non-classical methods for time-fractional derivatives.

As an important model problem for this approach we

consider a type of wave equation with time-fractional dampening related to acoustic waves in viscoelastic media with applications in the physics of medical ultrasound.

Minisymposium M9

Advances in solvers and preconditioning for PDE problems
Organisers
Niall Bootland and Sean Hon

Parallel preconditioning for the time-dependent Stokes problem

Andy Wathen *(University of Oxford)*

Block preconditioners for the Stokes problem that render this problem essentially as easy to solve as the Laplace problem were introduced by David Silvester and myself over 30 years ago. More recent concerns have focued on parallelisable solvers for time-dependent problems. After briefly reviewing the steady problem, we will here describe a recent parallel block preconditioning approach for the time-dependent Stokes problem.

This is joint work with Fede Danieli and Ben Southworth.

Symbol-based aggregated multigrid method for block Toeplitz linear systems

Matthias Bolten & Marco Donatelli & Paola Ferrari & **Isabella Furci** *(University of Genoa)*

We present a novel symbol-based multigrid procedure for solving large block Toeplitz linear systems. Our proposed method combines an aggregation-based strategy that transforms the symbol from matrix-valued to scalar-valued with standard grid transfer operators for scalar Toeplitz systems. This allows for the study of sufficient convergence conditions for grid transfer operators and smoothing parameters for scalar-valued functions, which are more computationally tractable. Indeed, contrary to existing methods, the only computation involving the matrix-valued symbol is its diagonalization when evaluated in a single point. We consider a block Jacobi smoother and we provide a rigorous proof of the smoothing property. Moreover, we ensure that the two-grid method converges proving the approximation property and we extend the convergence analysis to the V-cycle method. The numerical experiments show computational advantages of our method compared to existing methods for block Toeplitz linear systems.

A block α-circulant based preconditioned MINRES method for evolutionary partial differential equations

Sean Hon *(Hong Kong Baptist University)*

In this work, we propose a novel parallel-in-time preconditioner for an all-at-once system arising from the numerical solution of evolutionary partial differential equations (PDEs). Namely, considering the wave equation as a model problem, our main result concerns a block α-circulant matrix based preconditioner that can be fast diagonalized via fast Fourier transforms, whose effectiveness is theoretically supported for the modified block Toeplitz system arising from discretizing the concerned wave equation. Namely, after first transforming the original all-at-once linear system into a symmetric one, we develop the desired preconditioner based on the spectral information of the modified matrix. Then, we show that the eigenvalues of the preconditioned matrix are clustered around 1 without any extreme outlier far away from the clusters. In other words, mesh-independent convergence is theoretically guaranteed when the minimal residual method is employed. Moreover, our proposed solver is further generalized to a full block triangular Toeplitz system which arises when a high order discretization scheme is used. Numerical experiments are given to support the effectiveness of our preconditioner, showing that the expected optimal convergence can be achieved.
This is joint work with Xuelei Lin (Harbin Institute of Technology).

NFFT in Parameter Learning for Nonlocal Image Denoising Models

Andrés Miniguano-Trujillo[1] & John Pearson[2]
[1] *(Maxwell Institute for Mathematical Sciences)*
[2] *(University of Edinburgh)*

This work considers the numerical solution of a bilevel optimisation problem for the estimation of parameters in nonlocal image denoising models. The relevant parameters are the fidelity weight and a weight within the kernel of the nonlocal operator. Variational methods are used to characterise local minima via a first order optimality system. A finite element method is used to discretise the kernel and the associated linear

systems. For the former, a nonequispaced fast Fourier transform [1] is used to efficiently compute the vectorial Gauss transform associated with the nonlocal kernel as in [2]. For the latter, we use a preconditioner based on the nonlocal matrix to speed up the iterations of the LGMRES Krylov method. We use a second-order trust-region algorithm for optimising the denoising parameters. Several experiments are provided to illustrate the efficiency of the method and contrast them against the dense-matrix approximation showcased in the previous work [3].

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

Using spectral information for the robust solution of positive Maxwell problems via domain decomposition

Niall Bootland & Victorita Dolean & Frédéric Nataf & Pierre-Henri Tournier *(STFC Rutherford Appleton Laboratory)*

We consider the solution of linear systems arising from finite element discretisations of positive Maxwell problems using domain decomposition. In order to provide a robust solver, we design adaptive coarse spaces that complement a near-kernel space made locally from the gradient of scalar functions. The new class of preconditioner is inspired by the idea of subspace decomposition, but is based on spectral coarse spaces, and are specially designed for curl-conforming discretisations of Maxwell's equations in heterogeneous media. This extends results for the nodal auxiliary space preconditioner of Hiptmair and Xu to an approach that is further robust in the variable coefficient case and for non-convex domains at the expense of a larger coarse space. Numerical results will demonstrate the effectiveness of our approach even with the presence of many holes penetrating the domain, where the nodal auxiliary space preconditioner fails.

Minisymposium M10

PDEs in data science
Organisers
Lisa Maria Kreusser and Jonas Latz

PDE methods for joint reconstruction-segmentation of images

Jeremy Budd *(Universität Bonn/Caltech)* & Yves van Gennip *(TU Delft)* & Franca Hoffmann *(Caltech)* & Jonas Latz *(Heriot–Watt University)* & Carola-Bibiane Schönlieb *(University of Cambridge)* & Allen Tannenbaum *(Stony Brook University)*

In practical image segmentation tasks, the image must first be reconstructed from indirect, damaged, and/or noisy observations. Traditionally, reconstruction-segmentation would be performed in sequence: first reconstructing the image, then segmenting that reconstruction. Joint reconstruction-segmentation performs reconstruction and segmentation simultaneously, using each to guide the other.

Past joint reconstruction-segmentation has employed relatively simple segmentation algorithms, e.g. Chan–Vese. This talk will describe how joint reconstruction-segmentation can be performed using the more recent techniques of Bhattacharyya-flow-based segmentation (Michailovich *et al.*, 2007) and graph-PDE-based segmentation (Merkurjev *et al.*, 2013).

References

[1.] O.M ichailovich, Y. Rathi, and A. Tannenbaum, *Image segmentation using active contours driven by the Bhattacharyya gradient flow,* IEEE Transactions on Image Processing **16** (2007), pp. 2787–2801.

[2.] E. Merkurjev, T. Kostić, and A.L. Bertozzi. *An MBO scheme on graphs for classification and image processing*, SIAM Journal on Imaging Sciences **6**, no. 4 (2013), pp. 1903–1930.

A geometric view of adversarial machine learning

Leon Bungert & Nicolás García Trillos, Ryan Murray, Kerrek Stinson *(Technical University of Berlin)*

It is well-known that despite their aptness for complicated tasks like image classification, modern neural networks are prone to insusceptible input perturbations (a.k.a. adversarial attacks) which can lead to severe misclassifications. Adversarial training is a state-of-the-art method to train classifiers which are more robust against these adversarial attacks. The method features minimization of a robust risk and has interpretations as game-theoretic problem, distributionally robust optimization problem, dual of an optimal transport problem, or nonlocal geometric regularization problem. In this talk I will focus on the last interpretation which allows for the application of tools from calculus of variations and geometric measure theory to study existence, regularity, and asymp-

totic behavior of minimizers. In particular, I will show that adversarial training of binary classifiers is equivalent to a nonlocal and weighted perimeter regularization of the decision boundary. Furthermore, I will show Gamma-convergence of this perimeter and its discretization on a random geometric graph to a local anisotropic perimeter as the strength of the adversary tends to zero, thereby establishing an asymptotic regularization effect of adversarial training.

Modelling opinion formation in social networks with p-Laplacians on hypergraphs

Ariane Fazeny & Martin Burger & Daniel Tenbrinck *(Friedrich-Alexander-Universität Erlangen-Nürnberg)*

Traditional graphs are a versatile tool for encoding relationships between different entities and can hence be applied to image processing, machine learning or other mathematical problems. Oriented hypergraphs are a natural extension of traditional graphs, which also capture higher-order relationships instead of only allowing pairwise connections.

Therefore, we use oriented hypergraphs to model interactions on social networks and define gradient flows in the form of diffusion equations on hypergraphs to model information flow. In contrast to the traditional graph approach, we do not focus on pairwise interactions between individuals of the social network, but rather higher-order connections between multiple people and due to the more general structure of hypergraphs, we are able to model group dynamics, such as opinion formation, realistically and include so-called opinion leaders (individuals with a large following, who hence have great impact on the beliefs of others).

The introduced first-order differential operators and p-Laplacian operators on oriented hypergraphs are a valid generalization of the differential operators for traditional graphs and extend already existing definitions for the oriented hypergraph case such that the first eigenfunction is trivial and the second eigenfunctions therefore more easily interpretable.

Koopman-based spectral clustering of directed and time-evolving graphs

Stefan Klus *(Heriot–Watt University)*

While spectral clustering algorithms for undirected graphs are well established and have been successfully applied to unsupervised machine learning problems ranging from image segmentation and genome sequencing to signal processing and social network analysis, clustering directed graphs remains notoriously difficult. We will first exploit relationships between the graph Laplacian and transfer operators and in particular between clusters in undirected graphs and metastable sets in stochastic dynamical systems and then use a generalization of the notion of metastability to derive clustering algorithms for directed and time-evolving graphs. The resulting clusters can be interpreted as coherent sets, which play an important role in the analysis of transport and mixing processes in fluid flows. We will illustrate the results with the aid of guiding examples and simple benchmark problems.

Many-agent systems and mean-field models for semi-supervised learning

Lisa Maria Kreusser *(University of Bath)*

In many problems in data classification, it is desirable to assign labels to points in a point cloud where a certain number of them is already correctly labeled. In this talk, we propose a microscopic ODE approach, in which information about correct labels propagates to neighbouring points. Its dynamics are based on alignment mechanisms, often used in collective and consensus models. We derive the respective continuum description, which corresponds to an anisotropic diffusion equation with a reaction term. Solutions of the continuum model inherit interesting properties of the underlying point cloud. We discuss the qualitative behaviour of solutions and exemplify the results with micro- and macroscopic simulations.

Can Physics-Informed Neural Networks beat the Finite Element Method?

Jonas Latz & Tamara G. Grossmann, Urszula Julia Komorowska, Carola-Bibiane Schönlieb *(Heriot-Watt University)*

Partial differential equations play a fundamental role in the mathematical modelling of many processes and systems in physical, biological and other sciences. To simulate such processes and systems, the solutions of PDEs often need to be approximated numerically. The finite element method, for instance, is a usual standard methodology to do so. The recent success of deep neural networks at various approximation tasks has motivated their use in the numerical solution of PDEs. These so-called physics-informed neural networks and their variants have shown to be able to successfully approximate a large range of partial differential equations. So far, physics-informed neural

networks and the finite element method have mainly been studied in isolation of each other. In this work, we compare the methodologies in a systematic computational study. Indeed, we employ both methods to numerically solve various linear and nonlinear partial differential equations: Poisson in 1D, 2D, and 3D, Allen-Cahn in 1D, semilinear Schrödinger in 1D and 2D. We then compare computational costs and approximation accuracies. In terms of solution time and accuracy, physics-informed neural networks have not been able to outperform the finite element method in our study. In some experiments, they were faster at evaluating the solved PDE.

Corresponding preprint:
Grossmann, Komorowska, Latz, Schönlieb (2023): Can Physics-Informed Neural Networks beat the Finite Element Method? arXiv:2302.04107.

Correcting the Bias in Laplace Learning at Low Label Rates

Matthew Thorpe *(University of Manchester)*

Laplace learning is a semi-supervised method that finds missing labels via minimising a Dirichlet energy. It is well known that Laplace learning is (asymptotically) ill-posed at low labelling rates. In this talk I will identify the bias of Laplace learning and show how this can be corrected leading to significant improvement in performance. The correction in the bias leads one to a Poisson equation.

Computational Methods for Bayesian Imaging with Deep Gaussian Process Priors

Simon Urbainczyk & Jonas Latz, Aretha Teckentrup *(Heriot-Watt University)*

In image reconstruction, an accurate quantification of uncertainty is of great importance for informed decision making. Here, the Bayesian approach to inverse problems can be used: the image is represented through a random function that incorporates prior information which is then updated through Bayes' formula. Finding a prior is difficult. Images often exhibit non-stationary effects and multiscale behaviour. Thus, usual Gaussian process priors are not suitable. Deep Gaussian processes, on the other hand, encode non-stationary behaviour in a natural way through their hierarchical structure. To apply Bayes' formula, one commonly employs a Markov chain Monte Carlo method that requires sampling from the prior. In the case of deep Gaussian processes, sampling is especially challenging in high dimensions: the associated covariance matrices are large, dense, and changing from sample to sample. A popular strategy towards decreasing computational complexity is to view Gaussian processes as the solutions to a fractional stochastic partial differential equation (SPDE). In this work, we investigate efficient computational strategies to solve the fractional SPDEs occurring in deep Gaussian process sampling. Indeed, we employ rational approximations to represent the fractional operators through sparse matrices and reduce computational cost from cubic to near-linear. We test our techniques in standard Bayesian image reconstruction problems.

Discrete-to-continuum limits of graph-based gradient flows

Yves van Gennip & Yoshikazu Giga & Jun Okamoto *(Delft University of Technology)*

Gradient flows on graphs are common ingredients in machine learning methods. Discrete-to-continuum limits of such flows are of interest since they establish consistency of the method. In this talk we will have a look at the limits of two such flows: the total variation flow and the one-dimensional Allen–Cahn flow.

Minisymposium M11

Recent advances in multilevel, multiscale, and parallel in time methods

Organisers
Hussam Al Daal and Felix Kwok

Domain decomposition training strategies for physics-informed neural networks

Victorita Dolean *(University of Strathclyde) & Alexander Heinlein & Siddhartha Mishra & Benjamin Moseley*

Physics-informed neural networks (PINNs) are a solution method for solving boundary value problems based on differential equations (PDEs). The key idea of PINNs is to incorporate the residual of the PDE as well as boundary conditions into the loss function of the neural network. This provides a simple and mesh-free approach for solving problems relating to PDEs. However, a key limitation of PINNs is their lack of accuracy and efficiency when solving problems

with larger domains and more complex, multi-scale solutions. In a more recent approach, Finite Basis Physics-Informed Neural Networks (FBPINNs), the authors use ideas from domain decomposition to accelerate the learning process of PINNs and improve their accuracy in this setting. In this talk, we show how Schwarz-like additive, multiplicative, and hybrid iteration methods for training FBPINNs can be developed. Furthermore, we will present numerical experiments on the influence on convergence and accuracy of these different variants.

Preconditioners for mixed finite element problems based on element Schur complements

Tyrone Rees & Michael Wathen *(STFC Rutherford Appleton Laboratory)*

In this talk we introduce a generic approximation to Schur complements arising from inf-sup stable mixed finite element discretizations of self-adjoint multi-physics problems. In recent years 'natural-norm' preconditioning, where we infer the preconditioner from the function space on which the underlying problem is posed, has proved to be a successful approach. However, while powerful, this technique requires the user to have detailed knowledge of the mathematical formulation of their problem.

Our new approach builds a sparse approximation to a natural-norm preconditioner. It does this by explploiting the discretization mesh by forming local, or element, Schur complements and projecting them back to the global degrees of freedom. The resulting Schur complement approximation is sparse, has low construction cost (with the same order of operations as a general finite element matrix), and is amenable to off-the-shelf solution techniques, such as algebraic multigrid.

Using the LBB condition, we show that the preconditioned system has a favorable eigenvalue distribution. We present several numerical results to demonstrate the viability of this approach on a range of applications. Interestingly, numerical results show that the method gives an effective approximation to the non-symmetric Schur complement from the steady state Navier-Stokes equations.

Optimizing the Space-Time Multigrid algorithm for the heat equation

Bastien Chaudet-Dumas & Martin J. Gander & Ausra Pogozelskyte *(University of Geneva)*

For time-dependent problems, Parallel-in-Time (PinT) algorithms allow us to parallelize problems in the time dimension when space parallelization alone creates communication bottlenecks. Parareal and Multigrid Reduction-in-Time (MGRIT) are two examples of such PinT algorithms based on multigrid techniques, but they are not truly scalable since they coarsen the problem only in the time dimension.

We will focus on a more intrusive method: the Space-Time Multigrid algorithm with block-Jacobi relaxation introduced by Gander and Neumüller. This algorithm provides excellent scalability for parabolic problems up to millions of cores, while still being equally as fast as forward substitution on one core only.

We will show that the performance of this algorithm can be further improved by the optimization of the smoothing parameters. This will allow the algorithm to be up to twice as fast as the original one. Results will be presented for the heat equation discretized with Backward Euler.

A Super-Localized Generalized Finite Element Method

Philip Freese & Moritz Hauck & Tim Keil & Daniel Peterseim *(Hamburg University of Technology)*

We present a novel multi-scale method for solving elliptic partial differential equations with arbitrarily rough coefficients. The method constructs problem-adapted ansatz spaces with uniform algebraic approximation rates. Localized basis functions with the same super-exponential localization properties as the recently proposed Super-Localized Orthogonal Decomposition [M. Hauck, D. Peterseim, *Math. Comp. 92 (2023), 981-1003*] enable an efficient implementation. Stability of the basis is enforced by a partition of unity approach. We present a natural extension to higher order, resulting in higher approximation rates and enhanced localization properties. A rigorous a priori and a posteriori error analysis is performed, and we validate our theoretical findings in a series of numerical experiments, including challenging high-contrast coefficients.

Adaptively optimised Schwarz methods

Conor McCoid & Felix Kwok *(Université Laval)*

Optimised Schwarz methods use Fourier analysis to find transmission conditions between subdomains that provide faster convergence over standard Schwarz methods. However, this requires significant upfront analysis of the operator, and may not be straightforward for all problems. This work presents two black box methods for adaptively optimising the transmission conditions, one of which is equivalent to GMRES.

A Two-Level Domain Decomposition Method for Periodic Schrödinger Eigenstates in Anisotropically Expanding Domains.

Lambert Theisen & Benjamin Stamm *(University of Stuttgart)*

This talk presents a two-level domain decomposition method for the linear Schrödinger eigenvalue problem with periodic potentials for a non-uniform spatial expansion of the domain. In this framework, the numerical solution using inner-outer iterative eigenvalue algorithms suffers from a collapsing spectral gap that leads to deteriorating converge rates. We solve the collapsing gap problem by a quasi-optimal spectral-shift strategy to uniformly bound the number of iterations with respect to different domain sizes. Since the algorithm requires the solutions of shifted linear systems, we further propose a two-level decomposition method that includes the already computed spectral asymptotics in a suitable coarse space. This domain decomposition preconditioner is easy to construct, leads to a bounded condition number for the shifted linear systems, and efficiently utilizes the geometric subdivision of the domain. We test the method's robustness and efficiency numerically. If time permits, we analyze the method's scalability within the theoretical framework of spectral coarse spaces.

Minisymposium M12

Recent advances in the robust solution of singularly perturbed differential equations

Organisers

Niall Madden and Torsten Linß

POD approximations to the Navier-Stokes equations based on time derivatives

Julia Novo & Bosco García-Archilla & Volker John & Sarah Katz *(Universidad Autónoma de Madrid)*

In this talk we study reduced order methods based on proper orthogonal decomposition (POD) for approaching the incompressible Navier-Stokes equations. The set of snapshots is based on temporal derivatives of the velocity computed with a full order mixed finite element method (FOM). Including snapshots approaching the time derivative allow us to prove pointwise in time error bounds for the velocity. The set of snapshots contains also the mean velocity of the full order model. We add grad-div stabilization to the FOM and the POD model. With the aid of grad-div stabilization we are able to prove error bounds for the velocity and pressure approximations with constants independent of the Reynolds number.

Pressure and convection robust bounds for CIP-stabilized divergence-free elements for the Navier-Stokes equations

Bosco García-Archilla & Julia Novo *(Universidad de Sevilla)*

We analyze a continuous interior penalty (CIP) stabilization for discretizations of the incompressible Navier-Stokes equations using (divergence-free) Scott-Vogelius elements. This stabilization was recently introduced in [1] for steady Oseen (linear) equations, where the authors proved $O(h^{r+1/2})$ error bounds (h being the mesh diameter and r the degree of the piecewise polynomials used). We extend these error bounds to the time-dependent Navier-Stokes equations. The bounds are pressure-robust, meaning that the velocity does not depend on the pressure, and convection-robust, meaning that the constants in the error bounds do not depend on the Reynolds number.

References

[1.] G.R. Barrenechea, E. Burman, E. Cáceres, and J. Guzmán. Continuous interior penalty stabilization for divergence-free finite element methods, 2022

Raviart–Thomas-enriched Scott–Vogelius finite element methods for the Stokes equations on general meshes

Christian Merdon & Xu Li & Volker John *(WIAS Berlin)*

This talk concerns finite element methods for the incompressible Navier–Stokes problem that satisfy desirable structural properties like inf-sup stability,

pressure-robustness and exact preservation of the divergence constraint. Without pressure-robustness, complicated pressures can cause large errors in the velocity for small viscosities caused by a violation of the orthogonality between irrotational forces and divergence-free functions.

Traditional finite element methods do not satisfy the divergence constraint exactly with the exception of the Scott–Vogelius finite element methods, i.e., $P_k - P_{k-1}$ pairs, which are inf-sup stable on special meshes such as barycentric refined meshes. The talk discusses a new approach which stabilizes the Scott–Vogelius elements by enriching the velocity space with some specially chosen Raviart–Thomas functions on arbitrary shape-regular meshes, while maintaining the divergence-free property. Similar to other divergence-free methods, a reduction step is possible that results effectively in a $P_k - P_0$ discretisation.

The final part extends the new approach to the Navier–Stokes problem, where also the convection-robustness property is of importance and suitable discretizations of the nonlinear term are discussed.

Algebraic stabilizations of convection–diffusion problems and their convergence on general meshes

Petr Knobloch *(Charles University, Prague)*

Algebraically stabilized finite element discretizations of scalar steady-state convection–diffusion–reaction equations often provide accurate approximate solutions satisfying the discrete maximum principle (DMP). However, it was observed that a deterioration of the accuracy and convergence rates may occur for some problems if meshes without local symmetries are used. We investigate these phenomena both numerically and analytically and the findings are used to design a new algebraic stabilization called Symmetrized Monotone Upwind-type Algebraically Stabilized (SMUAS) method. The SMUAS method is linearity preserving and satisfies the DMP on arbitrary simplicial meshes. Moreover, we present numerical results indicating that the SMUAS method leads to optimal convergence rates on general simplicial meshes.

Parameter-Robust Discretizations and Solvers for Singularly Perturbed Problems on Curved Domains

Scott MacLachlan *(Memorial University of Newfoundland)* & Hisham bin Zubair & Muhammad Shahid

Recent years have seen continued progress in developing parameter-robust numerical methods for singularly perturbed PDEs, including both convection-diffusion and reaction-diffusion cases. Of particular note has been the development and application of advanced discretizations to these problems, yielding near-optimal error estimates in strong norms, as well as the development of boundary-layer preconditioners and advanced multigrid and domain-decomposition methods for these discretizations. In this talk, I will present recent work focused on expanding these results to domains beyond the unit square, including adapting existing multigrid methodology to the punctured domain of the Hemker problem.

Solving singularly perturbed problems using enriched finite element spaces

Niall Madden & Kirk Soodhalter *(University of Galway)*

Solutions to singularly perturbed problems often feature boundary and interior layers. Most standard finite element methods are based on polynomials spaces, which may fail to represent these layers in an adequate manner, unless a very fine mesh is used.

There have been numerous attempts to construct specialised numerical schemes that incorporate (*a priori*) information convening layer phenomena into the numerical method in order the compute solutions that are robust and layer-resolving. There is a rather extensive literature on fitted meshes relating to this.

Analogously, there have been efforts to develop specialised discretizations include layer-like terms in the discretization. Examples of these include the method proposed by Kellogg and Xenophontos, which involves enhancing a finite element space with layer-like terms [Int. J. Numer. Anal. Model. 7 (2010)]. The concept has a natural appeal, but there are computational draw-backs. For example, Giani proposes a minimization problem, to circumvent difficulties associated with ill-conditioning (and density) of the linear system [SIAM J. Sci. Comput. 40 (2018)]. Hong and Jung apply an enriched spectral method, where the FE space is enriched by functions satisfying a related reduced problem [J. Sci. Comput. 74 (2018)].

The approach we propose is principally motivated by the work of Kellogg and Xenophontos, but takes a novel view of analysis and implementation. We focus on linear reaction-diffusion problems. The resulting

scheme is shown to be stable and accurate, even when applied on a uniform grid.

Fitted finite element methods for reaction diffusion problems on Shishkin meshes

Alan F. Hegarty & Eugene O'Riordan *(University of Limerick & Dublin City University)*

Fitted finite element methods are constructed for a singularly perturbed reaction-diffusion problem in two space dimensions. Exponential splines as basis functions are combined with Shishkin meshes to obtain stable parameter-uniform numerical methods which satisfy a discrete maximum principle. We examine their convergence in the L^∞ norm for all values of the singular perturbation parameter.

Uniform convergence of an arbitrary order balanced FEM applied to a singularly perturbed shell problem

Torsten Linß *(FernUniversität in Hagen)* & Norber Heuer *(Pontificia Universidad Católica de Chile)*

We study a boundary value problem that describes the bending of an axisymmetrically loaded thin shell. The thickness of the shell appears in the differential equation as a singular perturbation parameter. As a consequence layers form and must be resolved by the numerical scheme.

We show that the energy norm naturally associated with the standard weak formulation fails to capture the layers. Using an idea by Lin and Stynes [1], we devise an alternative variational formulation whos induced norm (a so called "balanced norm") is stronger. This is then discretised using arbitrary order conforming FEM. We proof convergence on a layer-adapted mesh that is robust with respect to the perturbation parameter.

References

[1.] R. Lin and M. Stynes. A balanced finite element method for singularly perturbed reaction-diffusion problems. *SIAM J. Numer. Anal.*, 50(5):2729–2743, 2012.

Generation of layer-adapted meshes using mesh PDEs and numerical derivatives

Róisín Hill[*] & Niall Madden[†] *([*] University of Limerick, [†] University of Galway)*

We consider the numerical solution, by finite elements methods, of singularly-perturbed reaction-convection-diffusion equations whose solutions exhibit boundary layers. Our model problem is

$$-\varepsilon^2\Delta u + \mu\mathbf{b}\cdot\nabla u + cu = f, \in \Omega \subseteq \mathbb{R}^d, \quad \text{with } u|_{\partial\Omega} = 0, \tag{1}$$

where $d = 1, 2$. Here $\mathbf{b}, c$ and f are given functions with $c-(\text{div }\mathbf{b})/2 > 0$, $0 < \varepsilon \ll 1$ and $0 < \mu \leq 1$. Our interest lies in developing parameter-robust methods, where the quality of the solution is independent of the value of the perturbation parameter, ε. One way to achieving this is to use layer resolving methods based on meshes that concentrate their mesh points in regions of large variations in the solution.

We investigate the use of Mesh PDEs (MPDEs), based on Moving Mesh PDEs first presented in [1], to generate layer resolving meshes that yield parameter robust solutions to (1). Our chosen one-dimensional MPDE is

$$(\rho(x, u_h)x'(\xi))' = 0 \quad \text{for } \xi \in (0, 1), \tag{2}$$

and we impose boundary conditions that fix the end points of the resulting mesh. For (1) with $d = 1$, posed on the unit interval,

$$\rho(x, u_h) = \max\left\{1, K\left(|u_h'(x_0^+)|\exp\left(-\frac{|u_h'(x_0^+)|x}{\sigma}\right)\right.\right.$$

$$\left.\left.+|u_h'(x_N^-)|\exp\left(-\frac{|u_h'(x_N^-)|(1-x)}{\sigma}\right)\right)\right\}, \tag{3}$$

where K and σ are user-defined parameters. It should be noted that this formulation is independent of whether the solution to the related SPDE has one or two boundary layers or their location. The algorithms and code build on those presented in [3], but note that derivatives in (3) are estimated numerically and are applied to the numerical solution of reaction-convection-diffusion problems.

We then present generalisations of (2) to generate meshes for two-dimensional reaction-convection-diffusion problems. Implementations in FEniCS [2] are outlined.

References

[1.] W. Huang, Y. Ren, and R.D. Russell. Moving mesh partial differential equations (MMPDES) based on the equidistribution principle. *SIAM J. on Numer. Anal.*,31(3):709-730, 1994.

[2.] M.S. Alnæs, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M.E. Rognes, and G.N. Wells. The FEniCS project version 1.5. *Archive of Numerical Software*, 3(100), 2015.

[3.] R. Hill and N. Madden. Generating layer-adapted meshes using mesh partial differential equations, *Numer. Maths. Theory MethodsAppl.,* 14(3):559-588, 2021.

Minisymposium M13

Mathematical and Computational Foundations of AI

Organisers
Des Higham and Ivan Tyukin

Constrained and Multirate Training of Neural Networks

Tiffany Vlaar *(McGill University & Mila - Quebec AI Institute)*

I will describe algorithms for regularizing and training deep neural networks. Soft constraints, which add a penalty term to the loss, are typically used as a form of explicit regularization for neural network training. In this talk I describe a method for efficiently incorporating constraints into a stochastic gradient Langevin framework for the training of deep neural networks. In contrast to soft constraints, our constraints offer direct control of the parameter space, which allows us to study their effect on generalization. In the second part of the talk, I illustrate the presence of latent multiple time scales in deep learning applications. Different features present in the data can be learned by training a neural network on different time scales simultaneously. By choosing appropriate partitionings of the network parameters into fast and slow parts I show that our multirate techniques can be used to train deep neural networks for transfer learning applications in vision and natural language processing in half the time, without reducing the generalization performance of the model.

Elliptic PDE learning is provably data-efficient

Nicolas Boullé *(University of Cambridge)*, Diana Halikias, and Alex Townsend

PDE learning is an emerging field at the intersection of machine learning, physics, and mathematics, that aims to discover properties of unknown physical systems from experimental data. Popular techniques exploit the approximation power of deep learning to learn solution operators, which map source terms to solutions of the underlying partial differential equation (PDE). Solution operators can then produce surrogate data for data-intensive machine learning approaches such as learning reduced order models for design optimization in engineering and PDE recovery. In most deep learning applications, a large amount of training data is needed, which is often unrealistic in engineering and biology. However, PDE learning is shockingly data-efficient in practice. We provide a theoretical explanation for this behaviour by constructing an algorithm that recovers solution operators associated with elliptic PDEs and achieves an exponential convergence rate with respect to the size of the training dataset. The proof technique combines prior knowledge of PDE theory and randomized numerical linear algebra techniques and may lead to practical benefits such as improving dataset and neural network architecture designs.

Robust low-rank training via approximate orthonormal constraints

Dayana Savostianova[1] & Emanuele Zangrando[1] & Gianluca Ceruti[2] & Francesco Tudisco[1]
([1] Gran Sasso Science Institute, [2] EPF Lausanne)

With the fast development of Deep Learning, the size of the potentially solvable tasks has widely grown, alongside the corresponding models. To contrast the resulting increased demand for resources, a remarkable effort has been put into developing a variety of pruning methods. In order to reduce both inference and training costs, a prominent pruning strategy is to use low-rank matrix factorizations to represent the network weights. In this work, we observe that robustness, being already a critical problem in the DL field, can be compromised even more using available low-rank training methods. We argue that one of the possible causes is the explosive behavior of the singular values of the low-rank weight matrices. Thus, we introduce a robust low-rank training algorithm that maintains the network's weights on the low-rank matrix manifold while simultaneously enforcing approximate orthonormal constraints. The developed model reduces training and inference costs by staying on the low-rank manifold during training while keeping the accuracy of the original model, ensuring well-conditioning and, consequently, improved robustness. The reduced framework's performance in terms of accuracy and robustness is demonstrated for several benchmark classification datasets on commonly used

models.

Componentwise adversarial attacks

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

In today's world, deep neural networks have become the go-to tool for various classification tasks. They have shown state-of-the-art performance in many areas, from medical imaging to autonomous driving. However, they are also known to be vulnerable to adversarial attacks, which can cause misclassification by making small, imperceptible changes to the input image.

Adversarial attacks have become a serious concern in the development and deployment of deep learning models, particularly in safety-critical domains such as autonomous vehicles, medical diagnosis, and financial fraud detection. Recent research has shown that adversarial attacks can be carried out in various ways, including adding noise to the input data, modifying the structure of the model, and manipulating the training data.

To investigate this issue, we propose a novel approach based on backward error and condition number, which are concepts that have proved useful in numerical analysis. Specifically, we build on the work of Beuzeville et al. (2021) and develop a new class of attack algorithms that use componentwise relative perturbations. Such attacks are highly relevant in the case of handwritten documents or printed texts where, for example, the classification of signatures, postcodes, dates, or numerical quantities may be altered by changing only the ink consistency and not the background. This makes the perturbed images look natural to the naked eye. Such "adversarial ink" attacks therefore reveal a weakness that can have a serious impact on safety and security.

We illustrate the new attacks on MNIST and contrast them with state-of-the-art algorithms. We also study the use of a componentwise condition number to quantify vulnerability. Our findings show that the proposed approach can effectively generate adversarial examples that are difficult for deep learning models to classify correctly, while at the same time preserving the natural appearance of the original images.

On the extended Smale's 9th problem, phase transitions and the limits of trustworthy AI

Alexander Bastounis *(University of Leicester)* & Anders C. Hansen *(University of Cambridge)*

Instability and hallucinations are the Achilles' heel of modern AI and a paradox, with training algorithms finding unstable and hallucinating neural networks (NNs) despite the existence of stable and accurate ones. This prompts the fundamental question: can one build trustworthy AI?

This is now becoming a delicate question with connections to the regulation of AI technology in high risk areas. In this talk we discuss how this question is linked to recent results on the extended Smale's 9th problem, from the list of mathematical problems for the 21st century, and newly discovered phase transitions in optimisation. In particular, we will discuss how these results link to the difficulty of creating verification algorithms that can verify the validity of the output of modern AI.

The Limits of Verifiable Accuracy and Stability in Neural Networks

Ivan Y. Tyukin *(King's College London)* & Alexander Bastounis *(University of Leicester)* & Alexander N. Gorban *(King's College London)* & Anders C. Hansen *(University of Cambridge)* & Desmond J. Higham *(University of Edinburgh)* & Danil Prokhorov *(Toyota Tech Center)* & Oliver Sutton *(King's College London)* & Qinghua Zhou *(King's College London)*

In this talk, we consider the fundamental problem of determining whether a neural network with some fixed architecture can simultaneously and non-trivially show excellent generalisation and be stable and robust to data perturbations, adversarial or purely accidental. For cases when such networks exist we ask is it possible to verify that a given network has such properties. In addition, we are also interested in determining potential computational costs involved in verifying network's stability. We present a nested family of realistic neural network architectures for which both stable and unstable models may coexist within arbitrarily close proximity of each other in their corresponding parameter space, and for which determining robust generalisation involves computational costs which are exponential in the network's input dimension. The results, along with other relevant technical assumptions, could be used to guide the selection of neural architectures as a function of data dimensionality, data volumes, and margins of acceptable risks.

Geometry of Decision Boundaries and Robust-

ness in Deep Learning

Martin Lotz & Paul Lezeau *(University of Warwick)*

The sensitivity of neural networks to perturbations of the input - either adversarial or random - has been the subject of extensive work in the past years. We propose an approach to study the robustness of neural network classifiers via an analysis of the geometry of the decision boundaries in terms of the parameters and the structure of the neural network. Inspired by the probabilistic analysis of condition numbers in numerical analysis and optimization, the approach is based on bounds on tubular neighbourhoods of sets defined by Pfaffian functions.

When Algorithms Attack

Des Higham *(University of Edinburgh)*

Many commentators are asking whether current AI solutions are sufficiently robust, resilient, and trustworthy; and how such issues should be quantified and addressed. In an extreme case, it has been shown that a traffic "Stop" sign on the roadside can be misinterpreted by a driverless vehicle as a speed limit sign when minimal graffiti is added. The vulnerability of systems to such adversarial interventions raises questions around security and ethics, and there has been a rapid escalation of heuristic attack and defence strategies. I will show how a very simple scenario, accessible to analysis, reproduces effects that have been observed in practice when the input space is high dimensional: (i) the classification tool is guaranteed to be unstable, (ii) a standard gradient-based algorithm will find a perturbation that exploits this vulnerability, but (iii) the tool is robust to small random perturbations. The talk is based on joint work with Ivan Tyukin and Oliver Sutton (King's College London).

Minisymposium M14

Structure-preserving discretisations of Hilbert complexes

Organisers

Kaibo Hu and Deepesh Toshnival

Using complexes to preserve structures in fluid dynamics.

Marien Hanot *(IMAG, University of Montpellier)*

The goal of this presentation is to translate the essential conservation properties of fluid dynamics into the language of differential complexes. This translation is not one-to-one and, the preservation of conserved quantities will guide the selection.

As for the different choices we have, we can think of the choice of the degree of the form used to modelize the velocity, but it is not the only choice. Indeed, the discretizations of PDEs based on Hilbert complexes are generally based on the use of discrete subcomplexes. In order to preserve the structure of the continuous complex, these subcomplexes must be linked to it by projections commuting with the differential operator (or cohain morphism). This gives two possibilities for the projector going from the continuous to the discrete space: the cochain morphism or the L^2-orthogonal projection.

Although FEEC methods will often use the orthogonal projection, the cochain morphism also has interesting properties. We will show the consequences of this choice on the conservation properties. We will also sketch the other possibilities for the discretization brought by the use of the cochain map instead of the orthogonal projector, such as alleviating the necessity of using a discrete space which is a subspace of the continuous one.

Local bounded commuting projections for Hilbert complexes

Yizhou Liang & Jun Hu & Ting Lin *(University of Augsburg)*

We construct the local bounded commuting projection operators of nonstandard finite element de Rham complexes in two and three dimensions systematically. For three dimensions, the result can be applied to the standard de Rham complex, Hermite complex, Argyris complex and Neilan's complex. For two dimensions, the result can be applied to the Hermite-Stenberg complex and the Falk-Neilan complex. This result can be extended to the construction of the local bounded commuting projection operators to the discrete gradgrad complexes in two and three dimensions.

Bounded commuting projections for non-matching interfaces

Frederik Schnack & Martin Campos Pinto *(Max-*

Planck-Institute for Plasma Physics)

We present commuting projection operators on de Rham sequences of two-dimensional multipatch spaces with local tensor-product parametrization and non-matching interfaces. Our construction yields projection operators which are local and stable in any L^p norm with $p \in [1, \infty]$: it applies to locally refined shape-regular patches with different mappings, under the assumption that neighboring patches have nested resolutions and that interior vertices are shared by exactly four patches. Following a broken-FEEC approach, we first apply a tensor-product construction on the single-patch de Rham sequences and modify the resulting patch-wise commuting projections to enforce their conformity while preserving their commuting, projection, and stability properties with constants independent of both the size and the inner resolution of the individual patches.

Isogeometric Analysis and second-order complexes

Jeremias Arf & Bernd Simeon *(RPTU Kaiserslautern-Landau)*

The concept of Finite Element Exterior Calculus (FEEC), introduced by Arnold, Winther, and Falk, is an elegant and abstract framework for designing numerical methods for various partial differential equations (PDEs) related to Hilbert complexes and Hodge-Laplace operators. FEEC provides sufficient conditions for the well-posedness and convergence of discrete mixed weak formulations associated with the Hodge-Laplacians. Buffa et al. demonstrated that FEEC can be used in the context of Isogeometric Analysis (IGA), leading to structure-preserving discretizations of the classical de Rham sequence. While previous literature mainly focuses on first-order complexes like the de Rham chain, this talk deals with the use of IGA when a second-order complex underlies. We discuss the challenges that arise and study examples where a generalization is feasible. Theoretical considerations are exemplified by numerical tests, including the field of linear elasticity. The results show that the extension of FEEC to higher-order complexes in IGA might be a promising approach for the numerical treatment of PDEs.

Finite Element Complexes from Complexes

Xuehai Huang & Long Chen *(Shanghai University of Finance and Economics)*

Finite element complexes with various smoothness, including the de Rham complex, the Stokes complex, the curldiv complex, the Hessian complex, the elasticity complex, and the divdiv complex, are systematically constructed in this talk. First smooth scalar finite elements are developed based on a non-overlapping decomposition of the simplicial lattice and the Bernstein basis of the polynomial space. Smoothness at vertices and on edges are more than doubled than those on edges and on faces, respectively. Then the finite element de Rham complexes with various smoothness are devised using smooth finite elements with smoothness parameters satisfying certain relations. Finally, finite element Hessian complexes, finite element elasticity complexes and finite element divdiv complexes are derived from finite element de Rham complexes by using the Bernstein-Gelfand-Gelfand (BGG) framework. Dimension count and div stability play an important role for verifying the exactness of finite element complexes.

Boundary Element Exterior Calculus

Erick Schulz & Ralf Hiptmair *(Plexim)*

We report a surprising and deep structural property of first-kind boundary integral operators for Hodge–Dirac and Hodge–Laplace operators associated with de Rham Hilbert complexes on a bounded subdomain of a Riemannian manifold. We will show that from a variational perspective, those first-kind boundary integral operators are Hodge–Dirac and Hodge–Laplace operators as well, this time set in a trace de Rham Hilbert complex on the boundary whose underlying spaces of differential forms are equipped with non-local inner products defined through layer potentials. On the way to this main result, we will show how these layer potentials in operator-induced trace spaces can be developed and representation formulas will be presented. We will then discuss boundary element Galerkin discretization for the so-called Hodge-X operators and obtain gab-based a priori error estimates.

Fast computation of electromagnetic wave propagation with spline differential forms

Rafael Vázquez & Bernard Kapidani *(École Polytechnique Fédérale de Lausanne)*

We present an structure-preserving geometric method which exhibits high order of convergence and, contrarily to other high order geometric methods, does not

rely on the geometric realization of any dual mesh. The method is based on the De Rham complex of tensor-product B-splines, from which we construct two exact sequences of differential forms: the primal sequence starts from splines of degree p and at least C^1 continuity; the dual sequence starts from the space of tensor-product splines of degree $p-1$, which in the parametric domain coincides with the last space of the primal sequence.

The differential operators (gradient, curl and divergence) are condensed in the exterior derivative operator. They are well defined for both sequences, and can be expressed in terms of incidence matrices associated to a Cartesian mesh. The method is completed with two sets of discrete Hodge-star operators relating the two sequences, mapping the space of primal k-forms into the space of dual $(n-k)$-forms, and vice versa. The discrete Hodge-star operators encapsulate all the metric-dependent properties, including material properties, see [2].

We show a particular choice of the discrete Hodge-star operators inspired by [1] and how to compute them through the fast inversion of Kronecker product matrices. We apply the method to the solution of Maxwell equations for electromagnetic wave propagation [3]. The numerical tests confirm that the method conserves energy exactly, it has high order of convergence, and the computational cost is much lower than for standard Galerkin discretizations. We will also present preliminary results about the extension of the method to multi-patch geometries, going beyond the tensor-product structure.

References

[1.] R. Hiptmair. Discrete Hodge operators. *Numer. Math.*, 90:265–289, 2001.

[2.] Bernard Kapidani and Rafael Vázquez. High order geometric methods with splines: an analysis of discrete Hodge–star operators. *SIAM J. Sci. Comput.*, 2022.

[3.] Bernard Kapidani and Rafael Vázquez. High order geometric methods with splines: fast solution with explicit time-stepping for Maxwell equations. 2023. arXiv:2302/04979.

Minisymposium M15

Approximate computing in numerical linear algebra

Organisers

Nick Higham, Xiaobo Liu and Bastien Vieublé

Orthogonalization schemes in Tensor Train format

Martina Iannacito & Olivier Coulaud & Luc Giraud *(INRIA Center at the University of Bordeaux)*

In the framework of tensor spaces, we consider orthogonalization kernels to generate an orthogonal basis of a tensor subspace from a set of linearly independent tensors. In particular, we investigate experimentally the loss of orthogonality of six orthogonalization methods, namely Classical and Modified Gram-Schmidt with (CGS2, MGS2) and without (CGS, MGS) reorthogonalization, the Gram approach, and the Householder transformation. To tackle the curse of dimensionality, we represent tensor with low-rank approximation using the Tensor Train (TT) formalism, and we introduce recompression steps in the standard algorithm outline through the TT-rounding method at a prescribed precision. After describing the algorithm structure and properties, we illustrate experimentally that the theoretical bounds for the loss of orthogonality in the classical matrix computation round-off analysis results are maintained, with the unit roundoff replaced by the TT-rounding precision. The computational analysis for each orthogonalization kernel in terms of the memory requirement and the computational complexity measured as a function of the number of TT-rounding, which happens to be the computational most expensive operation, completes the study.

Accelerating DNN training at the arithmetic level: a mixed-precision perspective

Silviu-Ioan Filip *(INRIA Centre Rennes, France)*

With the increasing adoption of deep learning, particularly with embedded/edge computing scenarios and the increasing complexity of state-of-the-art DNNs, there is a vested interest in improving the cost/performance ratio of DNN training. To do so, one has to consider low-precision arithmetic (*e.g.* 8-bit and lower formats). Smaller data sizes can reduce the hardware

needed and can potentially improve memory footprint, bandwidth, and power.

The most compute-intensive stage of DNN training and inference is matrix multiplication. In this talk we will overview the state-of-the-art in the use of mixed-precision computing for DNN training acceleration and present some of our work in this space focusing on the impact of combining various fixed- and floating-point representations in the design of multiply-accumulate (MAC) units inside general matrix multiply (GEMM) accelerators. We will also go over some simulation tools that allow users to experiment with low and mixed precision arithmetic during DNN training.

Extending randomized low-rank approximation techniques to parameter-dependent problems

Hei Yin Lam & Daniel Kressner & Gianluca Ceruti *(École Polytechnique Féderale de Lausanne, Switzerland)*

Randomized algorithms are an increasingly popular approach for performing low-rank approximation and they usually proceed by multiplying the matrix with random dimension reduction matrices (DRMs). Applying such algorithms directly to a matrix $A(t)$ depending on a parameter t in a compact set $D \subset \mathbb{R}^d$ would involve multiplying different, independent DRMs for every t, which is not only expensive but also leads to inherently non-smooth approximations. In this talk, we propose to use constant DRMs, that is, $A(t)$ is multiplied with the same DRM for every t. The resulting parameter-dependent extensions of two popular randomized algorithms, the randomized singular value decomposition and the generalized Nyström method, are computationally attractive. Therefore, we provide a probabilistic analysis for both algorithms when using Gaussian random DRMs, it shows that our methods reliably return quasi-best low-rank approximations. Next, we propose an extension to the time-evolution of the low-rank approximation of solutions to matrix differential equations. The scheme constructs the time-dependent approximation of the range and co-range of the solution via multiplying with DRMs and obtains the low-rank approximation by the generalized Nyström's method. Numerical experiments illustrating the properties of the proposed randomized scheme are presented.

Mixed-precision Paterson–Stockmeyer method for evaluating matrix polynomials

Xiaobo Liu & Nicholas J. Higham *(University of Manchester)*

The Paterson–Stockmeyer method is an evaluation scheme for matrix polynomials with scalar coefficients that arise in many state-of-the-art algorithms based on polynomial or rational approximants, for example, those for computing transcendental matrix functions. We derive a mixed-precision version of the Paterson–Stockmeyer method that can be faster and use less memory than its fixed-precision counterpart while delivering the same level of accuracy.

Randomized Orthogonal Projection Methods for Krylov Subspaces Solvers

Edouard Timsit *(INRIA Paris)*

Randomization can be used to speed up the orthogonal projection step in Krylov solvers. Through a theoretical and numerical investigation, we show that Randomized Orthogonal Projection Methods (ROPMs) over the Krylov subspace produce quasi-optimal estimations. We detail the convergence of these algorithms, which rate is similar to that of deterministic methods for all matrices of our test set, with occasional spikes of the error.

The effect of approximate coarsest-level solves on the convergence of multilevel V-cycle methods

Petr Vacek & Erin C. Carson *(Charles University)* & Kirk M. Soodhalter *(Trinity College Dublin)*

Multigrid methods are frequently used when solving systems of linear equations, applied either as standalone solvers or as preconditioners for iterative methods. Within each cycle, the approximation is computed using smoothing on fine levels and solving on the coarsest level.

With growth of the size of the problems that are being solved, the size of the problems on the coarsest level is also growing and their solution can become a computational bottleneck. In practice the problems on the coarsest level are often solved approximately, for example by Krylov subspace methods or direct methods based on low-rank approximation; see, e.g., [Buttari et al., Numerical Linear Algebra with Applications (2022)]. The accuracy of the coarsest-level solver is typically determined experimentally in order to balance the cost of the solves and the total number of multigrid cycles required for convergence.

In this talk, we present an approach to analyzing the effect of approximate coarsest-level solves in the multigrid V-cycle method for symmetric positive definite problems. Based on these results, we discuss how the choice of the low-rank threshold parameter and finite precision arithmetic for the block low-rank direct solver on the coarsest level may affect the convergence of the V-cycle method. The results are illustrated through numerical experiments.

Minisymposium M16

Recent advances in numerical approximation of eigenvalue problems
Organisers
Fleurianne Bertrand, Daniele Boffi and Arbaz Khan

Least-Squares methods for eigenvalue problems

Fleurianne Bertrand & Daniele Boffi *(Technical University Chemnitz)*

In this talk, we discuss spectral properties of operators associated with the least-squares finite element approximation of elliptic partial differential equations. The convergence of the discrete eigenvalues and eigenfunctions towards the corresponding continuous eigenmodes is studied and analyzed with the help of appropriate L^2 error estimates. A priori and a posteriori estimates are proved.

Adaptive spectral projection based methods for the numerical solution of wave equations with memory

Luka Grubišić & Stefano Giani & Christian Engstrom *(University of Zagreb)*

We present a spectral projection based finite element method to numerically approximate the solution of the wave equation with memory. The adaptivity includes the control of both the approximation properties of the discretization space (mesh adaptivity) as well as the size of the computed spectrum (k-adaptivity). The meshes are refined using a residual based error estimator, while the size of the computed spectrum is adapted using the L_2 norm of the error of the projected data. We show that the approach can be very efficient and accurate. In our approach the spectral projections are numerically computed and the approximation of the solution of the time-dependent problem is given by a summation of terms that are the product of projections of the data and the inverse Laplace transform of scalar functions. We discuss the efficiency of the approach based on spectral projections when several time points are computed, and in the context of a case where the data or the kernel depend on a parameter.

DPG-approximation for eigenvalue problem

Henrik Schneider & Fleurianne Bertrand & Daniele Boffi *(Universität Duisburg-Essen)*

The discontinuous Petrov-Galerkin (DPG) method has been adopted for many problems of solving partial differential equations. It was constructed to find optimal discrete test functions to get optimal stability constants. As it is hard to compute the optimal test functions for every class of problems the practical DPG formulation was introduced, with easily computable test spaces which are arbitrary close to the optimal ones. The mixed formulation of the DPG method comes with a residual error estimator, which can be used for a hp adaptive scheme.

The DPG method is also a promising approach for the computation of eigenvalues. In fact, for the Laplace eigenvalue problem, the natural eigenvalue formulation introduced in [1] leads to optimal a priori convergence rates. More precisely, these results can be obtained showing that the conditions of the practical DPG and the ideas of the DPG* method [2] are leading to a a priori convergence theory. So like in the source problem, the residual forms a reliable and efficient error estimator.

Numerical results validate the theoretical results and show optimal convergence rates with the residual error estimator. The fact that no compatibility of the finite element spaces is required and that the DPG method presents a major advantage of using a weaker variational formulation makes it a promising approach for challenging problems. We will shortly discuss the application involving elastic structure [3].

References

[1.] F. Bertrand and D. Boffi and H. Schneider *DPG approximation of eigenvalue problems.* Comput. Methods Appl. Math., Vol. **23**, pp. 1–17 2023.

[2.] Demkowicz, L. and Gopalakrishnan, J. and Keith, B. *The DPG-star method.* Comput. Math. Appl., Vol. **79**, pp. 3092–3116, 2020.

[3.] F. Bertrand and H. Schneider *Superconvergence of DPG approximations in linear elasticity* accepted, M2AN, 2022.

On the computation of Maxwell's eigenvalues with nodal elements

Fleurianne Bertrand *(Technical University Chemnitz)* & **Daniele Boffi** *(KAUST)* & Lucia Gastaldi *(Brescia)*

We consider the finite element approximation of the eigenvalues and eigenfunctions of the resonant cavity associated with Maxwell's equations.

It is well known that with a standard Galerkin formulation the optimal convergence is achieved when edge elements are used.

Recent results on the approximation of the spectrum associated with finite element least squares formulations can be extended to the Maxwell eigenvalue problem. This is straightforward in two dimensions and more elaborate in three dimensions.

One might wonder if such results are also valid when nodal elements are used for the approximation of the electric field.

The aim of this talk is to give an answer to this question and to compare the numerical results with other schemes involving nodal elements.

Approximating Laplace eigenvalues of circular sectors using isogeometric mesh grading

Philipp Zilk & Thomas Apel *(University of the Bundeswehr Munich)*

It has been widely discussed in the literature that Isogeometric Analysis (IGA) produces better results than Finite Element Analysis for eigenvalue problems on rectangular domains in one, two and three dimensions when using higher-order methods [1, 3]. On the one hand, this is due to the fact that finite elements produce so-called optical branches, meaning that the upper part of the spectrum is approximated inaccurately, a phenomenon which does not appear when using isogeometric elements of maximal smoothness. On the other hand, the overall accuracy is improved as the approximation constant of maximally smooth spline spaces is superior to the one obtained with classical finite element spaces [4].

We examine how this improvement of the eigenvalue approximation can be extended to certain domains with singularities. Therefore, we consider the Laplace eigenvalue problem on a circular sector with a conical point in the center as our model problem. By considering the exact solutions, we discuss the singular behavior of the eigenfunctions in detail. Some of the resulting eigenfunctions have a singularity of type r^ν, thus the corresponding eigenvalues can not be approximated well with uniform refinement procedures. Mesh grading techniques help to recover the optimal convergence order and have been proven effective for multipatch discontinuous Galerkin IGA schemes [2]. We introduce a single patch approach based on a singular isogeometric mapping and illustrate optimal convergence order for the eigenfunctions and eigenvalues. Finally, we use maximally smooth NURBS of higher degrees in our approach and compare the spectral approximation accuracy to classical higher order finite element graded mesh schemes. To conclude the presentation, we show how the approximation of Laplace eigenvalues can be used for an application in the context of crack identification.

References

[1.] R.R. Hiemstra, T.J.R. Hughes, A. Reali, and D. Schillinger. "Removal of spurious outlier frequencies and modes from isogeometric discretizations of second- and fourth-order problems in one, two, and three dimensions". In: *Comput. Methods Appl. Mech. Engrg.* 387 (2021), Paper No. 114115, 43.

[2.] U. Langer, A. Mantzaflaris, S.E. Moore, and I. Toulopoulos. "Mesh grading in isogeometric analysis". In: *Comput. Math. Appl.* 70.7 (2015), pp. 1685–1700.

[3.] C. Manni, E. Sande, and H. Speleers. "Application of optimal spline subspaces for the removal of spurious outliers in isogeometric discretizations". In: *Comput. Methods Appl. Mech. Engrg.* 389 (2022), Paper No. 114260, 38.

[4.] E. Sande, C. Manni, and H. Speleers. "Explicit error estimates for spline approximation of arbitrary smoothness in isogeometric analysis". In: *Numer. Math.* 144.4 (2020), pp. 889–929.

Divergence-free discretisations of the Stokes eigenvalue problem

Umberto Zerbinati *(University of Oxford)* & Fleurianne Bertrand *(Technische Universität Chemnitz)* and

Daniele Boffi *(KAUST)*

Since its introduction by Franco Brezzi, the inf-sup condition has been the key instrument to analyse the stability of any saddle point discretisation. This is because the inf-sup is the necessary and sufficient condition for the well-posedness of a saddle point discretisation. Or is there? In the case of the source problem, there is no hope that one might escape the inf-sup condition but eigenvalue problems are a very different beast. Indeed now a day it is well known that the inf-sup condition is neither necessary nor sufficient when considering certain types of eigenvalue problems arising from saddle point discretisation. We explore the implication of a lack of inf-sup stability for finite element discretisation of the Stokes eigenvalue problem.

Recent advances in adaptive finite element methods for Stokes eigenvalue problems

Arbaz Khan *(Indian Institute of Technology Roorkee (IITR))*

Over the last few decades, the numerical analysis of the finite element method for eigenvalue problems has been of increasing interest because of various practical applications. Specifically, the a posteriori error analysis of eigenvalue problems using finite element approximations has been well developed. However, most results are for the Laplace eigenvalue problem and only a few papers consider the a posteriori error analysis for the Stokes eigenvalue problem. It is the aim of this talk to present the a posteriori error analysis for the Stokes eigenvalue problem based on two additional finite element discretizations which enable higher order approximations of Stokes eigenvalues.

Adaptive hybrid high-order method for guaranteed lower eigenvalue bounds

Ngoc Tien Tran & Carsten Carstensen & Benedikt Gräßle *(Friedrich-Schiller-Universität Jena)*

The higher-order guaranteed lower eigenvalue bounds of the Laplacian in the recent work by Carstensen, Ern, and Puttkammer [Numer. Math. 149, 2021] require a parameter $C_{\mathrm{st},1}$ that is found *not* robust as the polynomial degree p increases. This is related to the H^1 stability bound of the L^2 projection onto polynomials of degree at most p and its growth $C_{\mathrm{st},1} \propto (p+1)^{1/2}$ as $p \to \infty$. A similar estimate for the Galerkin projection holds with a p-robust constant $C_{\mathrm{st},2}$ and $C_{\mathrm{st},2} \leq 2$ for right-isosceles triangles. This talk considers a modified hybrid high-order (HHO) eigensolver with this new inequality that directly computes guaranteed lower eigenvalue bounds under the idealized hypothesis of exact solve of the generalized algebraic eigenvalue problem and a mild explicit condition on the maximal mesh-size in the simplicial mesh. A key advance is a p-robust parameter selection.

The analysis of the new method with a different fine-tuned volume stabilization allows for a priori quasi-best approximation and improved L^2 error estimates as well as a stabilization-free reliable and efficient a posteriori error control. The associated adaptive mesh-refining algorithm performs superior in computer benchmarks with striking numerical evidence for optimal higher empirical convergence rates.

Non-stabilized virtual element method for acoustic vibration and the discrete compactness property

Linda Alzaben & Daniele Boffi & Andreas Dedner & Lucia Gastaldi *(King Abdullah University of Science and Technology, University of Warwick, University of Brescia)*

We focus on analyzing the virtual element method (VEM) for the acoustic vibration problem using a non-stabilized formulation. The standard VEM discrete bilinear forms consist of two parts: a singular part maintaining consistency on polynomials and a stabilization form enforcing coercivity. The construction of the space proposed by [2] leads to a stiffness matrix that uses only the polynomial part and a mass matrix associated with a non-stabilized discrete bilinear form that is projected onto the VEM space. The study carried out demonstrates first the equivalence of the original problem to a mixed variational formulation. The analysis of [1] with the discrete compactness property [3] are the necessary tools for proving the convergence of the discrete solution operator. To evaluate the performance of the method and its ability to accurately solve the acoustic vibration problem using a non-stabilized formulation, several numerical tests were conducted using the Dune library [4] on different element structures.

References

[1.] Boffi D, Brezzi F, Gastaldi L. *On the convergence of eigenvalues for mixed formulations.* Annali della Scuola Normale Superiore di Pisa-Classe di Scienze. 1997;25(1-2):131-54.

[2.] Beirão da Veiga L, Mora D, Rivera G, Rodríguez

R.*A virtual element method for the acoustic vibration problem.* Numerische Mathematik. 2017 Jul;136(3): 725-63.

[3.] Boffi D. *Approximation of eigenvalues in mixed form, discrete compactness property, and application to hp mixed finite elements.* Computer methods in applied mechanics and engineering. 2007 Aug 1;196(37-40):3672-81.

[4.] Dedner A, Kloefkorn R, *Nolte M. Python bindings for the DUNE-FEM module.* Zenodo. doi. 2020 Mar;10.

Eigenproblems on Poincaré's Disk: Benchmark Problems and Error Estimates

Harri Hakula *(Aalto University)*

In this talk we discuss some interesting properties of the standard PDE eigenproblem

$$-\Delta u = \lambda u,$$

with $\Delta = \frac{1}{4}(1-x_1^2-x_2^2)^2 \left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right)$, where the computational domain is a subset of the Poincaré's disk $\mathbb{D}$. This setting with negative curvature space is common in quantum physics. The seminal work by Aurich and Steiner [1] presents configurations with high energy eigenmodes where no localisation can be observed. Here their results are replicated using *hp*-FEM equipped with auxiliary subspace error estimation [2]. We also consider standard geometric benchmark problems where the analytic solutions are known, including Pacman and annulus. With properly graded meshes exponential convergence of the lowest modes is demonstrated and the efficacy of the error estimation technique is verified.

The set of numerical experiments covers Dirichlet, Neumann, and periodic boundary conditions.

References

[1.] R. Aurich, F. Steiner, Statistical properties of highly excited quantum eigenstates of a strongly chaotic system, Physica D 64 (1993), 185–214.

[2.] S. Giani, L. Grubišić, H. Hakula, J.S. Ovall, A Posteriori Error Estimates for Elliptic Eigenvalue Problems Using Auxiliary Subspace Techniques, Journal Of Scientific Computing, 88 (3), 2021.

Minisymposium M17

Numerical methods for fully nonlinear partial differential equations

Organisers

Max Jensen and Iain Smears

Neural network schemes for solving first-order HJB equations

Olivier Bokanowski *(LJLL, Université Paris Cité)*, Xavier Warin *(EDF, France)* and Averil Prost *(INSA Rouen, Normandie)*

We are interested in the approximation of first-order Hamilton-Jacobi-Bellman equations, for average dimensions (e.g. 2 to 10). We focus on a deterministic optimal control problem with a maximum running cost functional, in a finite horizon context. We propose deep neural network approximations for Bellman's dynamic programming principle. This work follows the lines of Huré, Pham, Bachouch and Langrené (SIAM J. Numer. Anal., vol. 59 (1), 2021, pp. 525-557) where algorithms are proposed in a stochastic context. We develop a new approach in order to deal with the propagation of errors in the deterministic setting, where no diffusion is present in the dynamics. Our mathematical analysis gives an error estimate in an average (L1) norm. The study will be also illustrated on some academic numerical examples related to front propagations models in the presence of obstacle constraints, showing the relevance of the approach for average dimensions and for non-smooth value functions.

Efficient implementation of characteristic-based schemes on unstructured triangular grids

Roberto Ferretti & Simone Cacace *(Università Roma Tre)*

Using characteristics to treat advection terms in linear of nonlinear time-dependent PDEs leads to a class of schemes, e.g., semi-Lagrangian and Lagrange–Galerkin schemes, which preserve stability under large Courant numbers, and may therefore be appealing in many practical situations. Unfortunately, the need of locating the feet of characteristics may cause a serious drop of efficiency in the case of unstructured space grids, and thus prevent the use of large time-step schemes on complex geometries.

In this work, we first perform an in-depth analysis of the main recipes available for characteristic location, and propose a technique to improve the efficiency of this phase, using additional information related to the advecting vector field. Then, we adapt these ideas to the case of Hamilton–Jacobi equations, in which characteristics are selected via a minimum condition.

We also present numerical tests, confirming a clear improvement which make the unstructured case comparable to the structured one in terms of efficiency.

A least squares Hessian/Gradient recovery method for fully nonlinear PDEs in Hamilton–Jacobi–Bellman form

Omar Lakkis & Amireh Mousavi *(University of Sussex)*

Least-squares finite element recovery-based methods provide a simple and practical way to approximate linear elliptic PDEs in nondivergence form where standard variational approach either fails or requires technically complex modifications.

This idea allows the creation of efficient solvers for fully nonlinear elliptic equations, the linearization of which leaves us with an equation in nondivergence form. An important class of fully nonlinear elliptic PDEs can be written in Hamilton–Jacobi–Bellman (Dynamic Programming) form, i.e., as the supremum of a collection of linear operators acting on the unkown.

The least-squares FEM approach, a variant of the nonvariational finite element method, is based on gradient or Hessian recovery and allows the use of FEMs of arbitrary degree. The price to pay for using higher order FEMs is the loss of discrete-level monotonicity (maximum principle), which is valid for the PDE and crucial in proving the convergence of many degree one FEM and finite difference schemes.

Suitable functional spaces and penalties in the least-squares's cost functional must be carefully crafted in order to ensure stability and convergence of the scheme with a good approximation of the gradient (or Hessian) under the Cordes condition on the family of linear operators being optimized.

Furthermore, the nonlinear operator which is not necessarily everywhere differentiable, must be linearized in appropriate functional spaces using semismooth Newton or Howard's policy iteration method. A crucial contribution of our work, is the proof of convergence of the semismooth Newton method at the continuum level, i.e., on infinite dimesional functionals spaces. This allows an easy use of our non-monotone schemes which provides convergence rates as well as a posteriori error estimates.

Analysis and Numerical Approximation of Second-order Mean Field Game Partial Differential Inclusions

Yohance Osborne & Iain Smears *(University College London)*

Mean Field Games (MFG) are models for Nash equilibria of large population stochastic differential games. Under simplifying assumptions, these equilibria are described by nonlinear systems in which a Hamilton—Jacobi—Bellman (HJB) equation and a Kolmogorov—Fokker—Planck (KFP) equation are coupled. In the classical formulation of the MFG system, the advective term of the KFP equation involves a partial derivative of the Hamiltonian that is assumed to be continuous. However, in many cases of practical interest, the underlying optimal control problem may give rise to bang-bang controls, which typically lead to nondifferentiable Hamiltonians.

In this talk we present results on the analysis and numerical approximation of second-order MFG systems for the general case of convex, Lipschitz, but possibly nondifferentiable Hamiltonians. In particular, we propose a generalization of the MFG system as a Partial Differential Inclusion (PDI) based on interpreting the partial derivative of the Hamiltonian in terms of subdifferentials of convex functions. We prove the existence of unique weak solutions to MFG PDIs under a monotonicity condition similar to one that has been considered previously by Lasry & Lions. Moreover, we introduce a monotone finite element discretization of the weak formulation of MFG PDIs and present theorems on the strong convergence of the approximations to the value function in H^1-norm and the strong convergence of the approximations to the density function in L^q-norms.

Bound preserving finite elements for nonvariational problems

Tristan Pryer & Gabriel Barrenechea & Emmanuil Georgoulis *(University of Bath)*

The work presents a nonlinear finite element method for classes of nonvariational and fully nonlinear prob-

lem. The novelty of the method is that it guarantees bounds on the nodal values of the discrete problem match a priori bounds expected on the exact solution. We realise this constraint by introducing an appropriate nonlinear projection operator and seek the numerical solution within the range of this projection operator. The projection operator we use is not injective, hence stabilisation is required to ensure the well-posedness of the discrete problem.

To demonstrate the effectiveness of the proposed method, we showcase its application to linear nonvariational and fully nonlinear problems under Campanato-Cordes conditions. We establish near-best approximation results in mesh-dependent norms, specifically in an H^2 like norm, among all finite element functions that preserve the nodal bounds.

Gradient and Mirror Descent for Stochastic Control Problems

David Šiška *(University of Edinburgh)*

We study the convergence of Gradient and Mirror Descent schemes for approximating solutions to continuous-time stochastic control problems with measure-valued.

By exploiting Pontryagin Optimality Principle, these rely on solving forward and backward (adjoint) equations and performing static optimisation problems regularised with Bregman divergence and can be interpreted as implicit and explicit discretisations of the Fisher–Rao gradient flow. In the general (non-convex) case, we show that the objective function decreases along the gradient / mirror descent step. Moreover, in the convex / strongly convex case, when Pontryagin Optimality Principle provides a sufficient condition for optimality, we prove that the objective converges at the linear / exponential rate to its optimal value. The main technical difficulty is to show that stochastic control problem admits suitable relative smoothness and convexity properties. These are obtained by utilising the theory of Bounded Mean Oscillation (BMO) martingales required for estimates on the adjoint Backward Stochastic Differential Equation (BSDE).

This is joint work with Lukasz Szpruch and Bekzhan Kerimkulov.

Minisymposium M18

Simulating Stochastic Differential Equations

Organiser
Alix Leroy

The modified truncated Euler-Maruyama method for stochastic differential equations with concave diffusion coefficients

Yiyi TANG *(University of Strathclyde)*

The strong convergence theory of numerical solutions to stochastic differential equations (SDEs) was well studied under the global Lipschitz continuous condition. Recently, many researchers studied the strong convergence of numerical methods for SDEs with local Lipschitz continuous coefficients. For SDEs with polynomially growing coefficients, many new numerical methods were established, e.g., the truncated Euler-Maruyama (EM) method, the tamed EM method and so on. However, above numerical methods generally fail to work for SDEs whose coefficients are local Lipschitz near the zero. For this special challenge, an efficient numerical method is the drift implicit EM method. It covers many famous SDEs but it is an implicit EM method which means expensive computational cost. In addition, it only works for scalar SDEs. It may also fail to work for SDEs with superlinearly growing coefficients. In this talk, we will introduce the modified truncated EM method for multi-dimensional SDEs with superlinearly growing drift coefficients and concave diffusion coefficients.

Adaptive stepsize methods for weak approximation with Langevin dynamics

Alix Leroy *(Heriot-Watt University and University of Edinburgh)* & Jonas Latz *(Heriot-Watt University)* & Ben Leimkuhler *(University of Edinburgh)* & Des Higham *(University of Edinburgh)*

The work focuses on weak approximation of stochastic differential equations and develops a method of computing solutions of Langevin dynamics using variable stepsize. The method assumes a knowledge of the problem allowing to establish of a good 'monitor function' which locates points of rapid change in solutions of stochastic differential equations. Using time transformation we show that it is possible to integrate a rescaled system using fixed-stepsize numerical dis-

cretization effectively placing more timesteps where needed.

Abstracts of Contributed Talks

A nodally bound preserving finite element method for the convection-diffusion-reaction equation

Abdolreza Amiri & Gabriel R. Barrenechea *(University of Strathclyde)* Tristan Pryer *(University of Bath)*

It is well-known that the finite element (FE) Galerkin approximation of the convection-diffusion problem in the convection-diffusion regime generates highly oscillatory results, and additional numerical stabilization must be introduced. The most common stabilization methods are adding nonconsistent terms, e.g., homogeneous artificial diffusion or a penalty term called stabilization term to the discretization problem (Galerkin method). But even using stabilization does not guarantee the preserving of the *Discrete Maximum principles (DMP)* and/or *monotonicity properties*. Monotonicity implies positivity preservation which more generally indicates the bound preservation of the numerical solution, and is a weaker property than the DMP.

In our research, we extent the method proposed in the recent paper [1] to design a bound-preserving finite element scheme for the convection-diffusion-reaction equation.
Following the same line as in [1], we use the following property: There is a correspondence between the imposition of bounds on the numerical solution and searching for the numerical solution on a convex subset of the finite element space consisting of the discrete functions satisfying those bounds at their nodal values. So, we first project the finite element solution onto the subset of admissible finite element functions (that is, those that respect the bounds of the continuous problem). To remove the non-trivial kernel that appears as a result of this process, two stabilization terms are added to the discretized equations. One of those penalises the kernel (or "negative part" of the finite element solution), while the other one is aimed at increasing the stability of the method. We prove stability and optimal order error estimates for the method, and present numerous numerical experiments showcasing the applicability of the method to approximate problems with layers.

References

[1.] G.R. Barrenechea, E. Georgoulis, T. Pryer, A. Veeser, A nodally bound-preserving finite element method, arxiv.org/abs/2304.01067.

Novel conformal finite element error estimates for fourth order nonlinear Rosenau—Burger's model

Ankur & Ram Jiwari *(Indian Institute of Technology Roorkee)*

We design and implement a new conformal finite element error analysis to simulate the following fourth-order nonlinear Rosenau—Burger's model in two-dimensional case:

$$v_t + \Delta^2 v_t - \alpha\Delta v + \nabla\cdot\vec{\mathbf{1}}v + \vec{\mathbf{1}}v.\nabla v = 0 \quad \text{in } \Omega\times(0,T],\ T>0,$$

with appropriate initial and boundary conditions. Also, $\Omega \subseteq \mathbb{R}^n$ with n $\leq$ 2, $\alpha \geq 0$ and $\vec{\mathbf{1}} = (1,1)$. Here, the major challenge arises in designing a numerical method for fourth order problem.

The key feature of the proposed work is to provide priori error estimates in both L^2 and L^∞ Bôchner spaces simultaneously. To achieve the desired error estimates for discretized schemes, our idea is to introduce the appropriate projection operator that allows us to use the known estimates in the formulation of the desired results. Also, the stability, existence, and uniqueness in the most precise normed spaces have been established. Finally, the work is supported by numerical experiments to validate the developed theory, and graphically represent the wave phenomena.

Discretisation of viscoelastic fluid flows using the generalised Lie derivative

Ben Ashby *(Heriot-Watt University)*

Viscoelastic fluid models extend the Navier-Stokes equations by including an extra contribution to the stress tensor, depending upon the *conformation tensor*, σ, which is given by a constitutive law coupled to the fluid. In this work, we focus on the discretisation of differential constitutive laws for the conformation tensor, which are formulated in terms of the *upper-convected time derivative*, given by

$$\frac{\partial}{\partial t}\sigma + (u\cdot\nabla)\sigma - (\nabla u)\sigma - \sigma(\nabla u)^T$$

where u is the fluid velocity. This describes the rate of change of σ as it is advected and deformed by the fluid. Typically, these laws are hyperbolic PDEs, and

their numerical solution remains a challenge. A key point is that the physics of the problem dictate that the conformation tensor must remain positive definite for all flows, and violation of this condition often leads to numerical blowup.

In this talk, we present a full discretisation of the creeping flow of an Oldroyd-B fluid using the generalised Lie derivative approach. In this framework, the upper-convected derivative can be understood as a Lie derivative with respect to the flow via the deformation gradient tensor. Approximation of this derivative directly along flow characteristics allows all of its terms to be treated as one, rather than for example discretising the convective terms and deformation terms separately. We present numerical results at moderate Weissenberg number which demonstrate that the scheme is relatively cheap while preserving flow structure.

Towards a monolithic multigrid method for Oseen problems

Pierre-Loïc Bacq* & Yvan Notay† (* *(Université Paris-Saclay)* † *(Université Libre de Bruxelles)*

We consider the numerical solution of discrete Oseen problems. These problems naturally arise when linearizing Navier-Stokes problems with the Picard method and are challenging to solve[1]: as far as we know, no linear-time method can robustly solve them in a number of iterations bounded independently of the mesh size and of the Reynolds number, especially for variable convective flows. In particular, algebraic multigrid (AMG) methods often struggle with such problems because of the small or null pressure block [2].

In this talk, we will present a new approach introduced in [4] based on a simple algebraic transformation of the corresponding linear system which has already given good results for Stokes problems[3]. First, we describe the norm-based algebraic convergence theory for the two-grid method applied to the transformed system. For constant coefficient problems discretized by finite differences, we show that the convergence is indeed independent of both the mesh size, the Reynolds number and the orientation of the convection flow. To obtain this result, unsmoothed aggregation is used and aggregates of both velocity and pressure unknowns should be aligned in the direction of the convective flow.

Our second contribution is a semi-algebraic multigrid method which is applied to the transformed system. This method is intended for problems with variable convective flow. Information is used from the discretization to build an auxilary matrix, from which the aggregation of the pressure unknowns is algebraically determined. The aggregation of the velocity unknowns is algebraically determined from the velocity block of the system matrix. Numerical results show that the two-grid method converges independently of the mesh size and of the Reynolds number for constant convective flows, and almost independently of the Reynolds number for variable flows.

Finally, we explain the main difficulty encountered when extending the two-grid method to a multigrid one: the aggregation aligned with the direction of the convective flow introduces an anisotropy at the coarse levels which degrades the convergence. We then describe two ways to avoid this difficulty along with their advantages and limitations.

References:

[1.] S.A. Melchior, V. Legat, P. Van Dooren, and A.J. Wathen, Analysis of preconditioned iterative solvers for incompressible flow problems, Int. J. Numer. Meth. Fluids, 68 2012, pp. 269–28

[2.] M. Benzi, G.H. Golub, and J. Liesen, Numerical solution of saddle point problems, Acta Numer. 14 (2005), pp. 1–137

[3.] Y. Notay, Algebraic multigrid for Stokes equations, SIAM J. Sci. Comput. 39 (2017), pp. S88–S111

[4] P.-L. Bacq and Y. Notay, A new semi-algebraic two-grid method for Oseen problems, SIAM J. Sci. Comput. (2022), pp. S226-S253

High-Order Finite Element Schemes for the Stokes—Onsager—Maxwell Equations

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

In this talk we consider the Stokes—Onsager—Stefan–Maxwell (SOSM) equations, which model the flow of concentrated mixtures of distinct chemical species in a common thermodynamic phase. The equations account for both the diffusive interactions between chemical species and the bulk convection. Our aim is to develop computationally efficient high-order finite element schemes that discretize these nonlinear equations in two and three spatial dimensions. Because the SOSM equations relate many unknown variables (e.g. the bulk and species velocities, pressure, concentrations, chemical potentials, etc.), this is a difficult

task. In particular, there are many choices of which variables should be explicitly solved for in the formulation, and it is not clear which discrete finite element function spaces should be employed. To tackle this challenge, we derive a novel weak formulation of the SOSM problem in which the species mass fluxes are treated as unknowns. We show that this new formulation naturally leads to a large class of high-order finite element discretizations that are straightforward to implement and have desirable linear-algebraic properties. Moreover, from a theoretical standpoint, we are able to prove that when applied to a linearized version of the SOSM problem, the proposed finite element schemes are convergent. Our findings are illustrated with numerical experiments.

Performance analysis of FEM implementations in Matlab for arbitrary dimensions

Stefanie Beuter & Stefan Funken *(Ulm University)*

The finite element method has become a widespread tool for the approximation of solutions of partial differential equations. While the method allows for an application in many use cases, its performance depends on various factors. We present our efficient implementation in any space dimension and analyze the most performance crucial steps. The code covers all four steps of the adaptive FEM, namely SOLVE, MARK, ESTIMATE, and REFINE. The calculation of the linear system of equations is asymptotically the most time-consuming part. This can partly be caught by highly efficient solvers for sparse matrices, which has been subject to intensive studies in literature. As a result, the, sometimes recursively defined, refinements and the assembly of the problem matrix are additional crucial parts of the adaptive FEM. The latter problem has been addressed in several implementations by [1]–[9] in 2 and 3 dimensions. We discuss the different approaches and their advantages and disadvantages and compare them to our own general implementation. Hereby, several differences such as the problem dimension, object-oriented approaches, and the allowance of higher polynomial degrees for the ansatz space are considered. Important indicators of the routines are their performance in time depending on the problem size and their adaptability to new problems. While the calculation of the error estimator and marking are comparably small parts of the code in terms of performance, the second part to pay attention to is the refinement procedure. We realize a newest vertex bisection in arbitrary dimension. As for all three other steps of the adaptive FEM we implemented the refinement independent of the dimension. Therefore, no code changes are necessary, if problems of different dimensions are realized.

Since MATLAB has proven its strength in the realization of numerical simulation and partial differential equations over the years, all implementations are given in MATLAB. However, our code does not strongly depend on language specifics and is also given in Julia. Besides, it can easily be transferred to other vector languages.

References

[1.] S. Bartels: Numerical approximation of partial differential equations. In: *Springer* vol. 64, (2016)

[2.] L. Chen: iFEM: an innovative finite element method package in MATLAB. In: *Preprint, University of Maryland*, (2008)

[3.] L. Chen: Programming of finite element methods in matlab. In: *Arxiv*, (2018)

[4.] F. Cuvelier, C. Japhet, G. Scarella: An efficient way to assemble finite element matrices in vector languages. In: *BIT Numerical Mathematics* vol. 56, (2016)

[5.] S. Funken, D. Praetorius, P. Wissgott: Efficient implementation of adaptive P1-FEM in Matlab. In: *Computational Methods in Applied Mathematics*, (2011)

[6.] A. Hannukainen, M. Juntunen: HJfem_lite. In: *MATLAB Central File Exchange*, `https://www.mathworks.com/matlabcentral/fileexchange/36108-hjfem_lite`, Retrieved March 2, 2023.

[7.] M. Innerberger, D. Praetorius: MooAFEM: An object oriented Matlab code for higher-order adaptive FEM for (nonlinear) elliptic PDEs. In: *Arxiv* (2022)

[8.] J. Koko: Fast MATLAB assembly of FEM matrices in 2D and 3D using cell-array approach. In: *International Journal of Modeling, Simulation, and Scientific Computing*, (2016)

[9.] T. Rahman, J. Valdman: Fast MATLAB assembly of FEM matrices in 2D and 3D: Nodal elements. In: *Applied mathematics and computation*, (2013)

Deflated Gauss-Newton Methods

Alban Bloor Riley *(University of Manchester)*

Objective functions with many local minima are one of the biggest obstacles to finding the global mini-

mum of non linear least squares problems. In this talk we will discuss two deflated Gauss-Newton methods designed to systematically find all local minima of a problem, and thus the global minima. We will then cover the application of these methods to inverse eigenvalue problems associated with inelastic neutron scattering.

This is joint work with Marcus Webb (University of Manchester) and Mike Baker (Dept Chemistry, University of Manchester).

Computation of the pseudospectral boundary of unbounded operators

Lyonell Boulton & Catherine Drysdale *(Heriot-Watt University)*

The pseudospectrum is nowadays a well established tool for the analysis of linear operators, thanks to the tremendous success of the classical monograph of Trefethen and Embree [2], and the significant impact of the seminal work of Davies, which includes his influential monograph [1]. Methods for computing pseudospectra of matrices are widely available and have been sufficiently tested for about 30 years. By contrast, much less in known about methods for determining pseudospectra of operators on infinite dimensional spaces. For the latter, only a handful of reasonably well understood analytical techniques for construction of quasimodes, the implementation of Shur tests and the use of generalised Birman-Schwinger principles, are currently available. Moreover, these only apply to specific types of operators.

For general unbounded operators, an obvious idea is to consider finite-dimensional subspaces of the domain, find the pseudospectral boundaries of the associated projected matrices via any of the standard packages, then argue that these curves converge to the boundaries of the infinite model as the dimension of the subspaces increases. Unfortunately, even when this convergence is guaranteed, finding reliable information about the structure of the original curves by means of this approach is not straightforward. The pseudospectral boundaries of the matrix sections are closed compact curves, while usually those of the operator are unbounded curves, obeying a certain asymptotic behaviour at infinity. Determining which points of the matrix pseudospectrum reliably provide information about this asymptotic behaviour is often very difficult.

In this talk, we consider an adaptive method to detect and certify boundary points of the pseudospectrum of the operator. We formulate this method, so it can be implemented widely and reliably, in order to assess where to "cut the curve" of the matrix approximation. We show tests of this method on a simple, but non-trivial problem, first considered in [3]. As it turns, the proposed approach appears to detect true portions of the pseudospectral boundary of the operator, in realistic computational time. It also seems to give accurate estimates of the asymptotic behaviour expected for the pseudospectral boundary curve at infinity, at low computational cost.

References

[1.] E.B. Davies, *Linear Operators and Their Spectra* Cambridge University Press, Cambridge, 2007.

[2.] L.N. Trefethen and M. Embree, *Spectra and Pseudospectra* Princeton University Press, Princeton and Oxford, 2005.

[3.] *Journal of Fluid Mechanics*, Volume 497, 25 December 2003 , pp. 201 - 224.

Higher Order Far-Field Boundary Conditions for Crystal Defects Computations

Julian Braun & Christoph Ortner & Yangshuai Wang & Lei Zhang *(Heriot-Watt University)*

Lattice defects in crystalline materials create long-range elastic fields that can be modeled on the atomistic scale. The low rank structures of defect configurations are revealed by a rigorous far-field expansion of the long-range elastic fields, and thus the defect equilibrium can be expressed as a sum of continuum correctors and discrete multipole terms both of which are computable. We develop a novel family of numerical schemes that exploit the multipole expansions to accelerate the simulation of crystalline defects. To enclose the simulation in a finite domain, a theoretically justified approximation of elastic multipole tensors is introduced, which leads to a novel moment iteration resulting in higher order boundary conditions. Several prototypical numerical examples of point defects are presented to test the convergence for both geometry error and energy error. The numerical results show that our proposed numerical scheme matches the accelerated convergence rates in terms of computational cell size given by the rigorous convergence estimates.

Stochastic Bilevel Optimization

Ivan Cheltsov *(University of Bath)*

In the field of smooth bilevel optimization, existing deterministic algorithms, based on implicit differentiation of the inner problem, such as HOAG (2), have been effectively used to solve problems in areas such as hyperparameter optimization. These algorithms, however, exhibit a high per-iteration complexity, in large part due to the inversion of a hessian matrix, that takes place during the implicit differentiation stage. To tackle this issue, various algorithms have been developed, that, on the one hand, introduce stochasticity when solving the inner and outer problems, and on the other, use stochastic subroutines to invert the hessian in sub-$\mathcal{O}(n^3)$ time. We will introduce one such algorithm in particular - stocBIO (1). This algorithm, albeit having one of the fastest convergence rates among comparable algorithms, requires the tuning of a large number of parameters. We will begin the presentation with an explanation of the algorithm and state how it compares to the deterministic HOAG algorithm. We will discuss the benefits and drawbacks of the algorithm, as well as its existing modifications, such as MRBO and VRBO (4).

In the second part, we introduce a new subroutine for the Hessian inversion, based on the Implicit SGD algorithm, that demonstrates increased stability over the existing Neumann series subroutine (3), present in most of the current stochastic bilevel algorithms, including stocBIO.

References

[1.] Ji, K. Yang, J. & Liang. Y. Bilevel optimization: Convergence Analysis and Enhanced Design. *International Conference on Machine Learning (ICML)*, 2021.

[2.] Pedregosa, F. Hyperparameter optimization with approximate gradient. *Proceedings of The 33rd International Conference on Machine Learning, PMLR* 48:737-746, 2016. Available from https://proceedings.mlr.press/v48/pedregosa16.html.

[3.] Toulis, P., Horel, T., Airoldi, EM. (2020). The proximal Robbins-Monro method. Journal of the Royal Statistical Society, Series B

[4.] Yang, J., Ji, K., & Liang, Y. (2021). Provably Faster Algorithms for Bilevel Optimization. *Advances in Neural Information Processing Systems* (pp. 13670–13682). Curran Associates, Inc.

A comparison of two templates for three level discrete schemes

Raimondas Čiegis *(Vilnius Gediminas Technical University)*

In this talk we consider two templates for construction and analysis of three level discrete schemes (see also [1]):

$$B_h \frac{y^{m+1}-y^{m-1}}{2h_t} + h_t^2 R_h \Lambda_t y + A_h y = \varphi(t^m), \quad (1)$$

and

$$B_h(\rho\Lambda_t y) + \sigma h_t^2 A_h \Lambda_t y + A_h y = \varphi(t^m), \quad (2)$$

$$B_h(\rho\delta_t v^0) + \sigma h_t^2 A_h \delta_t v^0 + \frac{1}{2} h_t A_h v^0 = u_1 + \frac{1}{2} h_t \varphi^0.$$

They are used to construct and analyse new high-order compact finite difference schemes for the variable coefficient multidimensional wave equations

$$\rho(x)\partial_t^2 u(x,t) - (a_1^2\partial_1^2 + \ldots + a_n^2\partial_n^2)u(x,t) = f(x,t) \quad (3)$$

$$(x,t) \in Q_T = \Omega \times (0,T).$$

As an example of new general high-order scheme we present the following discrete scheme, which approximates the 3D PDE and initial conditions

$$\bar{s}_N(\rho\Lambda_t v) + \frac{1}{12} h_t^2 A_N \Lambda_t v + A_N v = f_N, \quad (4)$$

$$\bar{s}_N(\rho\delta_t v^0) + \frac{1}{12} h_t^2 A_N \delta_t v^0 + \frac{1}{2} h_t A_N v^0 = u_{1N} + \frac{1}{2} h_t f_N^0$$

where

$$\bar{s}_N := \prod_{k=1}^{n} s_{kN}, \quad s_{kN} := I + \frac{1}{12} h_k^2 \Lambda_k.$$

The stability and convergence estimates for the solution of (4) follow directly from general results obtained for the template (2).

Numerical examples supporting our theoretical analysis are provided and discussed.

References

[1.] A. Zlotnik, R. Čiegis. On Construction and Properties of Compact 4th Order Finite-Difference Schemes for the Variable Coefficient Wave Equation. *J. Sci. Comput. (2023) 95:3 https://doi.org/10.1007/s10915-023-02127-3*

Computation and Certification of the Pseudospectral Boundary

Catherine Drysdale & Lyonell Boulton *(University of Birmingham)*

The pseudospectrum is a well-established tool for the analysis of linear operators, often demonstrating important factors such as the sensitivity to perturbation of the eigenvalues [1]. Efficient calculation of the pseudospectrum for unbounded operators in infinite dimensional spaces is a relatively unexplored territory. Often finite-dimensional subspaces are used in place of the infinite dimensional space. In particular, the use of finite dimensional subspaces changes the qualitative nature of pseudospectral contours from unbounded curves with asymptotic behaviour at infinity to closed loops. The overlap between these curves forms the well resolved parts of the pseudospectrum, meaning parts of the spectrum with no spectral pollution. Therefore, it is useful to have a certification process for these calculated points. Especially, when computations on finite domains are used to support asymptotic results.

In this talk, we demonstrate an adaptive method to reliably follow the boundary points of the pseudospectrum of the operator. We test this method on a simple, yet challenging model that has been used to explore the dynamics of thin film of viscous fluid on the interior surface of a rotating cylinder. In the literature, the pseudospectral contours are expected to be asymptotic to parabolas [2], symmetric to the real axis centred at the origin. We adapt the linear operator to a Fourier Basis and then apply a curve tracing algorithm. With the curve-tracing algorithm, we only consider relevant parts of the domain. New points are accepted by the algorithm into the pseudospectral curve based on their passing a certification check. The certification check consists of calculating the singular value testing whether is within a tolerance of the desired contour level value as the number of Fourier modes increases up to a threshold. A different threshold is required in different parts of the domain and has to be specified beforehand. Additionally, the algorithm can be adapted for computational efficiency in comparison to traditional methods.

References

[1.] L.N. Trefethen and M. Embree, Spectra and Pseudospectra Princeton University Press, Princeton and Oxford, 2005.

[2.] Journal of Fluid Mechanics, Volume 497, 25 December 2003, pp. 201–224.

Row Replicated Block Cimmino

Iain Duff & Philippe Leleux, Daniel Ruiz, Sukru Torun *(Cerfacs, Toulouse)*

The block Cimmino method is a hybrid method for the solution of large sparse systems of equations. Although the basic Cimmino algorithm can be very slow as it is just using Jacobi's method on the normal equations, there are many ways to improve this algorithm to obtain a competitive method while retaining the high parallelism of Jacobi's method.

The blocks are obtained by a partitioning algorithm and subproblems on these blocks can be solved by a sparse direct method yielding a hybrid direct-iterative solver. the iteration equations can be solved by block conjugate gradients and recently we have used partitioning techniques that are numerically aware to increase the angles between the subspaces and reduce the number of iterations.

These previous algorithms generate disjoint partitions but in the current work we allow overlapping between the blocks. We show that this can decrease the overall time for solution and then show how the relationship of our work to overlapping domain decomposition enables us to define more targeted overlapping for domain decomposition that appears to be very competitive.

Approximating sparse Hessian matrices using large-scale linear least squares

Jaroslav M. Fowkes & Nicholas I.M. Gould *(STFC Rutherford Appleton Laboratory)* & Jennifer 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 have limitations. To try and overcome these, we propose a novel approach that reformulates the problem as the solution of a large linear least squares problem. The least squares problem is sparse but can include a number of rows that contain significantly more entries than other rows and are regarded as dense. We exploit recent work on solving such problems using either the normal matrix or an augmented system to derive a robust approach for computing approximate sparse Hessian matrices. Example sparse Hessians from the CUTEst test problem collection for optimization illustrate the effectiveness and robustness of the new method.

Multiscale Finite Element methods for an Elliptic Optimal Control Problem with Rough Coefficients and Control Constraints

José Garay & Susanne C. Brenner & Li-yeng Sung *(University of Augsburg)*

The solution of multi-scale elliptic problems with non-separable scales and high contrast in the coefficients by standard Finite Element Methods (FEM) is typically prohibitively expensive since it requires the resolution of all characteristic lengths to produce an accurate solution. Numerical homogenization methods such as Localized Orthogonal Decomposition (LOD) methods provide access to feasible and reliable simulations of such multi-scale problems. These methods are based on the idea of a generalized finite element space whose basis functions are obtained by modifying standard coarse standard FEM basis functions to incorporate relevant microscopic information in a computationally feasible procedure. Using this enhanced basis one can solve a much smaller problem to produce an approximate solution whose accuracy is comparable to the solution obtained by the expensive standard FEM. We present a variant of the LOD method that utilizes domain decomposition techniques and its application in the solution of an elliptic optimal control problem with rough coefficients and control constraints.

A fully discrete hypocoercivity-preserving Galerkin method

Philip J. Herbert & Emmanuil H. Georgoulis *(Heriot-Watt University)*

In this talk, we will discuss the recent developments in the topic of discretisations for so-called hypocoercive equations. We will focus our attention on the classical Kolmogorov equation which serves as a sufficiently rich model problem of kinetic equations with degenerate diffusion. Degeneracy of the diffusion prevents the application of the classical energy-type arguments which are typically used for the approximation of parabolic problems. Utilising a methodology which is novel to numerical methods, we are able to provide error estimates for a fully discrete scheme which uses discontinuous elements for the time discretisation and C^1 conforming elements for the spatial discretisation.

Stability of space-time boundary element methods for 1D wave problems.

D. Hoonhout & C.A. Urzúa-Torres *(Delft University of Technology)*

In this talk, we study when standard low-order BEM leads to discrete inf-sup conditions for both first kind and indirect second kind boundary integral equations (BIE) in 1D. Moreover, when the discrete inf-sup condition is violated, we present simple regularisations. Although additional numerical error is introduced, the use of these regularisations recovers unique solvability, preserves the expected asymptotic convergence rate, and is computationally considerably cheaper than the modified Hilbert transform. These results give us further understanding related to unstable behaviour sometimes observed in 1D, and pave the way towards computationally cheaper stable space-time BEM for the wave equation in higher dimensional problems.

References

[1.] O. Steinbach, C. Urzúa-Torres, A new approach to space-time boundary integral equations for the wave equation (2021).

[2.] O. Steinbach, C. Urzúa-Torres, M. Zank, Towards coercive boundary element methods for the wave equation, *In: arXiv*, (2021)

[3.] O. Steinbach, M. Zank, Coercive space-time finite element methods for initial boundary value problems, *Electron. Trans. Numer. Anal.*, **52**:154-194 (2020)

Preconditioned Iterative Methods for Structure-Preserving Discretisations

James Jackaman & *Scott MacLachlan* (NTNU, Norway)

In recent years, there has been substantial work on the development of so-called "structure-preserving" discretisations of differential equations, where the numerical approximation reflects key conservation laws observed of the continuum solution. While such discretisations are unquestionable valuable in situations where physical relevance and fidelity are closely tied to the conservation laws, their practical utility is limited by the fact that standard iterative methods for solution of the resulting linear and nonlinear systems only resolve the underlying conserved quantities when solved to near-machine precision. In this talk, we present a generalisation of the (preconditioned) flexible GMRES algorithm that can preserve arbitrarily many such conserved quantities exactly at (nearly) any stopping tolerance, with a small additional cost. Numerical results are presented for several structure-preserving finite-element discretisations of linear

parabolic and hyperbolic model problems.

Efficient Adaptive Stochastic Collocation Strategies for Advection-Diffusion Problems with Uncertain Inputs

Benjamin Kent & Catherine Powell & David Silvester & Malgorzata Zimoń *(University of Manchester)*

Physical models with uncertain inputs are commonly represented as parametric partial differential equations (PDEs). That is, PDEs with inputs that are expressed as functions of parameters with an associated probability distribution. Developing efficient and accurate solution strategies that account for errors on the space, time and parameter domains simultaneously is highly challenging. Indeed, it is well known that standard polynomial-based approximations on the parameter domain can incur errors that grow in time. In this work, we focus on advection–diffusion problems with parameter-dependent wind fields. A novel adaptive solution strategy is proposed that allows users to combine stochastic collocation on the parameter domain with off-the-shelf adaptive timestepping algorithms with local error control. This is a non-intrusive strategy that builds a polynomial-based surrogate that is adapted sequentially in time. The algorithm is driven by a so-called hierarchical estimator for the parametric error and balances this against an estimate for the global time-stepping error which is derived from a scaling argument.

Scaling to semi-doubly stochastic form

Philip A. Knight & Luce le Gorrec, Sandrine Mouysset, Daniel Ruiz *(University of Strathclyde)*

The Sinkhorn-Knopp algorithm (SKA) is a very well known way of scaling a square nonnegative matrix into a doubly stochastic matrix. SKA, and (faster) variants, have proven to be useful in a wide variety of applications (machine learning, bioinformatics, matching, etc). While it is impossible for a non-square nonnegative matrix to have row and column sums both equal to one, SKA can be adapted to scale rectangular matrices to prescribed row and column sums, assuming such scalings exist. We present a new generalisation of doubly stochastic matrices with particular relevance to rectangular matrices, which we christen "semi-doubly stochastic" (SDS). A nonnegative matrix A is SDS if A^TA and AA^T are doubly stochastic.

In contrast to doubly stochastic matrices, SDS matrices need not have support. We look at the implications in terms of the block structure of SDS matrices and show that so long as a rectangular matrix has the same nonzero pattern as an SDS matrix then it can be scaled to SDS form. While the block structure of semi-scalable matrices looks attractive, as this clearly has applications in co-clustering, there is no easy way to tell a priori whether a matrix has this property or not. In practice, if we attempt to use current scaling algorithms on such matrices without preexisting knowledge of the underlying block structure, then they will fail to converge to anything meaningful. To remedy this, we present a new iterative scaling algorithm related to SKA. We show the potential of a variant based on a Newton iteration. For an efficient implementation of the Newton step we need to solve a singular system implicitly to find a minimum norm least squares solution. We discuss techniques for circumventing potential pitfalls with this approach.

Analyzing Convergence of Schwarz Waveform Relaxation Methods Using Exponential Weighting

Felix Kwok & Alejandro Alfonso Rodriguez *(Université Laval, Canada)*

Schwarz waveform relaxation (SWR) is a family of domain decomposition methods for solving time dependent PDEs iteratively. The spatial domain is first decomposed into subdomains, and the time-dependent subdomain problems are solved in parallel, before interface data for the whole time interval are exchanged; the process is then repeated until convergence. SWR methods are known to converge superlinearly for bounded time intervals. However, to obtain sharp convergence estimates, one often needs to compute complicated inverse Laplace transforms, and for some interface conditions, there are no known formulas for the inverse transforms. In this talk, we show how exponential weighting techniques can be used to produce superlinear estimates without having to compute the inverse Laplace transforms explicitly. We will use this technique to analyze the convergence of SWR with Dirichlet and Robin transmission conditions.

Parallel-in-time solver for the all-at-once Runge–Kutta discretization

Santolo Leveque *(Scuola Normal Superiore)* & Luca Bergamaschi & Ángeles Martínez & John W. Pearson

Time-dependent PDEs arise very often in many sci-

entific areas, such as mechanics, biology, economics, or chemistry, just to name a few. Of late, many researchers have devoted their effort in devising parallel-in-time methods for the numerical solution of time-dependent PDEs. As opposed to the classical approach, in which an approximation of the solution at a time t is computed by a sequential time-stepping, parallel-in-time methods approximate the solution of the problem for all times concurrently. This in turns adds a new dimension of parallelism and allows to speed-up the numerical solution on modern supercomputers.

In this talk, we present a fully parallelizable preconditioner for the all-at-once linear system obtained when employing a Runge–Kutta method in time. The resulting system is solved iteratively for the numerical solution and for the stages of the method. By employing classical saddle-point theory, one is able to derive an optimal preconditioner for the system considered. This results in a block-diagonal solve for all the stages at all the time-steps, and a Schur complement obtained by solving again systems for the stages of the method. Since at each linear iteration one has to solve for the latter system, we introduce a new block-preconditioner based on the SVD of the (real) Runge–Kutta coefficient matrix $A_{\mathrm{RK}} = U\Sigma V^\top$.

A range of numerical experiments validate the robustness of the preconditioner with respect to the discretization parameters and to the number of stages, as well as very promising scalability and parallel efficiency indices.

Obtaining Pseudo-inverse Solution With MINRES and Preconditioned MINRES

Yang Liu *(University of Oxford)* & Andre Milzarek *(The Chinese University of Hone Kong, Shenzhen)* & Fred Roosta *(The University of Queensland)*

The celebrated minimum residual method (MINRES) was originally designed for solving linear least-squared problems involving Hermitian matrices. However, MINRES is not guaranteed to obtain the pseudo-inverse (minimum-length) solution unless the right-hand-side vector lies in the range of the underlying matrix. By introducing a novel lifting strategy, we propose a method to obtain such solution. We further extend a similar lifting strategy for MINRES variants that use positive semi-definite (PSD) matrices as preconditioners. The preconditioners are shown to result in dimensionality reduction. We also extend our methods to solve systems involving complex symmetric matrices. Numerical experiments are provided to support our analysis.

Block Preconditioners for the Implicit-in-Time Immersed Boundary Method

Gautam Luhana & Chen Greif *(University of British Columbia)*

The Immersed Boundary (IB) method is a popular method for simulating fluid-solid interactions. The IB method was initially designed by Charles S. Peskin to simulate fibrous heart valves, and has since evolved into a general-purpose method for simulating various types of solid dynamics immersed within a fluid. The key idea, and the reason for its popularity, is to keep the solid and fluid variables on two separate, Lagrangian and Eulerian, domains. The two grids communicate forces and velocities via integral operators with Dirac Delta kernels. This allows for simplicity in the code as well as avoids the problem of regeneration of the mesh resulting from deformations and movements of the solid structure.

Implicit schemes for the IB method have been around for a while but the real challenge has been to develop a scheme that is computationally competitive with the explicit schemes. The usual approach for the implicit IB method is to either eliminate the Lagrangian variables and solve the fully Eulerian system or vice versa. The first approach leads to a familiar 2×2 block Saddle-Point system that is difficult to solve efficiently due to the eulerian structural force term.

We propose an alternative approach of solving the full 3×3 block Double Saddle-Point system and present efficient and scalable preconditioners based on recent work on Double Saddle-Point systems. The preconditioners are based on LDU block factorizations and we present efficient approximations for the resulting Schur Complements.

A priori and a posteriori error analysis for semilinear problems in liquid crystals

Ruma R. Maity & Apala Majumdar, Neela Nataraj *(Aalto University)*

In this talk, we discuss finite element approximation of the nonlinear elliptic partial differential equations associated to a Landau-de Gennes model for nematic liquid crystals and ferronematic model. We establish existence and local uniqueness of the discrete solutions, a priori error estimates in the energy norm, and

a posteriori error estimates that steer the adaptive refinement process. The theoretical results are complemented by the numerical experiments on the discrete solution profiles, and the numerical convergence rates that corroborates the theoretical estimates.

Stochastic θ finite difference for a class of stochastic partial differential equations with applications to financial modelling

Walter Mudzimbabwe *(Johannesburg, South Africa)*

In this talk, we consider a class of stochastic partial differential equations (SPDEs) of the form

$$\mathrm{d}v = -\mu\frac{\partial v}{\partial x}\mathrm{d}t + \frac{1}{2}\frac{\partial^2 v}{\partial x^2}\mathrm{d}t - \sqrt{\rho}\frac{\partial v}{\partial x}\mathrm{d}W_t,$$

where W_t is a standard Brownian motion and μ and $0 \leq \rho \leq 1$ are real-valued parameters. We consider the solution of the SPDE as generalised stochastic differential equations (SDEs) and seek a numerical method of it. We then develop a numerical solution of the (SPDEs) as a composite scheme which combines an implicit and explicit Milstein numerical solution for the (SDE). We then consider the mean square stability conditions that the composite scheme must satisfy. Theoretic results of these stability conditions using Fourier analysis shows that the composite method is stable under certain conditions that are dependent on μ and ρ. We also confirm that the stability conditions of the stochastic finite difference scheme extend in an expected way from the deterministic partial differential equations (PDEs) stability conditions. To demonstrate the effectiveness of our results, we apply the results to a basket of credit derivatives.

On a shock capturing finite volume method that can solve fully incompressible flows

Michael Ndjinga & Esteban Coiffier *(Université Paris-Saclay and CEA Saclay)*

In Computational Fluid Dynamics, finite volume methods are often specifically designed for shock waves [3, 7], low Mach flows [1], or incompressible flows [2]. However, in an industrial context, the flow can include both high Mach and low Mach regions and transition in time between the two regimes. Furthermore the engineer may want to simulate a fully incompressible flow, for instance when the fluid equation of state is not easily available.

We propose a new finite volume discretisation that can precisely capture shock waves in high Mach flows, and is well defined when the fluid is assumed incompressible, ie where the Mach number is everywhere exactly zero.

This new method is strongly inspired by implicit in time finite volume schemes on staggered grids that were historically designed for incompressible flows [2]. These staggered discretisations are popular among multiphase flow engineers for their correct low Mach number asymptotic expansion [6]. However, they are generally non conservative, and their stability analysis has historically been performed with a heuristic approach and the tuning of numerical parameters [5]).

In this talk we study the connection between the numerical diffusion operator on one hand and both the low Mach number precision and checkerboard oscillations on the other hand.

We then propose a new conservative linearly L^2-stable finite volumes schemes for both compressible and incompressible fluid models. Unlike [4], our scheme is based on a carefully chosen numerical diffusion operator and the proof of stability follows from the symmetrisation of the system. An important remark is that unlike Godunov type schemes, the numerical diffusion operator of a symmetric system is not symmetric. This property is fundamental to ensure low Mach precision and avoid spurious checkerboard modes oscillations.

We give numerical results showing the good behaviour of the method in 1D and 2D for incompressible flows, low Mach and high Mach number flows, including shock waves.

References

[1.] S. Dellacherie. Analysis of Godunov type schemes applied to the compressible Euler system at low mach number *J. Comp. Phys.*, 229(4), pp. 978–1016, 2010.

[2.] J.W.F. Harlow. Numerical calculation of time-dependent viscous incompressible flow with free surface. *Physics of Fluids*, vol 8, pp. 2182–2189, 1965.

[3.] S.K. Godunov. A difference scheme for numerical solution of discontinuous solution of hydrodynamic equations. *Mat. Sbornik.* 47: 271–306, 1959.

[4.] R. Herbin, W. Kheriji and J.-C. Latché. On some implicit and semi-implicit staggered schemes for the shallow water and Euler equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, EDP Sciences, 48 (6), pp.1807–1857, 2014.

[5.] C.W. Hirt. Heuristic stability theory for finite difference equations. *J. Comp. Phys.*, 2, pp.339–355, 1968.

[6.] A. Prosperetti and G. Tryggvason. *Computational methods for multiphase flow.* Cambridge University Pres, 2009.

[7.] P.L. Roe. Approximate Riemann solvers, parameter vectors and difference schemes. *J. of Comput. Phys.*, 43, 357, 1981.

A decoupled and unconditionally convergent nodal projection free integrator for the Landau-Lifshitz-Gilbert equation including magneto striction.

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

We consider the coupled system of the Landau-Lifshitz-Gilbert (LLG) equation and conservation of momentum to describe magnetic processes in ferromagnetic materials including magnetostrictive effects. 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 magnetostriction.

PDE Constrained Optimisation for Brachytherapy Treatment Planning

Jennifer Power & Tristan Pryer *(University of Bath)*

Radiation therapy is among the most common methods for treating cancer. An essential aspect of the treatment process is the planning stage. Clinicians carefully create treatment plans to ensure the radiation is directed at the tumour, and not at the healthy tissue.

Brachytherapy is a cancer treatment where radioactive seeds are surgically implanted directly onto the tumour and slowly emit radiation, killing the tumour from the inside. A challenge lies in positioning the radioactive seeds such that the tumour receives the required dose, but healthy tissue is not exposed to excessive radiation.

This talk will discuss developing the brachytherapy treatment planning problem to obtain the optimal configuration of radioactive seeds. The problem is formulated as a PDE-constrained optimisation problem. The PDE constraint is given by a diffusion approximation to the Boltzmann transport equation. Additional constraints are imposed on the control variable to ensure that the radiation source remains positive, and that the source function is a specific shape. The problem is solved numerically using a Galerkin finite element method.

Numerical approximation of two dimensional variable order fractional differential equations

Shahzad Sarwar & Muhammad Yousuf *(King Fahd University of Petroleum and Minerals, Saudi Arabia)*

Variable-order fractional partial differential equations have been researched in a variety of modern applications in science and engineering. For example, Glockle and Nonnenmacher investigated the relaxation processes and reaction kinetics of proteins given by fractional differential equations, where the order of the derivative varies with temperature. Electroviscous or electrorheological fluids and polymer gels have been shown to modify their characteristics in response to variations in the strength of an applied electric field. Magnetorheological elastomers' characteristics respond to magnetic field strength. Damage modeling has revealed that when damage accumulates (over time) in a structure, the nonlinear stress/strain behavior changes. Variable-order calculus may be a better fit for this behavior. One challenging task in the study of fractional differential equations is to find the exact solution. In most cases, we do not know the exact solution for the problem and one needs to seek a numerical approximation. In this study, we consider the variable order fractional diffusion problem in two dimensions. A high order numerical scheme is proposed which is based on approximations of a matrix exponential function. Convergence order is higher than the existing algorithms. Finally a numerical example is given to verify the numerical algorithm.

Acknowledgement: The author acknowledges the funding support to attend this conference provided by the Deanship of Research Oversight and Coordination (DROC) at King Fahd University of Petroleum

& Minerals (KFUPM), Kingdom of Saudi Arabia.

Tensor product algorithms for Bayesian inference of networks from epidemiological data

Dmitry Savostyanov & Sergey Dolgov *(University of Essex)*

Epidemiological modelling is crucial to inform healthcare policies and to support decision making for disease prevention and control. The recent outbreak of COVID-19 pandemic raised a significant scientific and public debate regarding the quality of the mathematical models used to predict the effect of the pandemics and to choose an appropriate response strategy. To accurately capture how the disease spreads, we have to move beyond a usual assumption that the population is connected homogeneously (well–mixed), and towards network models of epidemics. Unfortunately, their complexity grows exponentially with the size of the network — these models suffer from the curse of dimensionality and usually rely on further approximations to make them practically solvable. In this talk we discuss how epidemiological models on networks can be solved accurately using the recently proposed algorithms based on low–rank tensor product factorisations. We also discuss the inverse problem of inferring a contact network from epidemiological data, for which we employ Bayesian optimisation techniques.

This is joint work with Sergey Dolgov (University of Bath, UK). This work is supported by the Leverhulme Trust Research Fellowship RF-2021-258.

Global Sensitivity Analysis of Pollutant Dispersion Uncertainty Quantification Problem

Tasnia Shahid *(University of Strathclyde)*

Air pollution is a pressing issue challenging modern society from both public health and environmental perspectives. The latest World Health Organisation (WHO) data shows that more than 90% of the world population "breathes air that exceeds WHO guideline limits" and each year 4.2 million deaths can be linked to ambient air pollution. Therefore, the measurement of air quality has become an important subject in metrology.

The use of computational modelling enables us to study pollutant dispersion models over a range of parameter values in order to gain some insight into the factors that strongly influence the pollution concentration present in the air. We study this through the use of a parametric advection-diffusion pollution dispersion model with parameters sampled from probability distribution functions to investigate how the pollutant concentration varies with respect to uncertainty in the model parameters. Hence, we investigate the pollutant dispersion model as an uncertainty quantification (UQ) problem.

We conduct a global sensitivity analysis (GSA) of the UQ pollutant dispersion problem in order to assess how the variability in the pollutant concentration can be attributed to the variability in the model parameters. This draws to attention the relative influence of each physical process in the pollutant dispersion model to the model output. We study this using a variance-based GSA technique called Sobol indices. We are interested in analysing Sobol indices across the problem domain to gain a better understanding of how the sensitivity of the solution to the parameters varies with respect to physical space.

The spatial sensitivity maps obtained could be used in an optimal placement strategy for sensors.

Uniform and unitary rational approximations of the matrix exponential

Pranav Singh *(University of Bath)* & Tobias Jawecki *(Vienna University of Technology)*

The exponential function maps the imaginary axis to the unit circle and for many applications this unitarity property is also desirable from its approximations. We show that this property is conserved not only by the (k,k)-rational interpolant of the exponential on the imaginary axis, but also by (k,k)-rational barycentric approximants that minimize a linearized approximation error. These results are a consequence of certain properties of singular vectors of Loewner-type matrices associated to linearized approximation errors. Prominent representatives of this class are rational approximants computed by the adaptive Antoulas–Anderson (AAA) method and the AAA–Lawson method. Our results also lead to a modified procedure with improved numerical stability of the unitarity property and reduced computational cost. Rational approximants generated by these approaches lead to an improved method for computing the matrix exponential of skew-Hermitian matrices, which has applications in the solutions of dispersive PDEs such as the Schrödinger equation. In particular, when the 'relevant' spectrum is small or split into smaller components, matrix exponential methods based on AAA and AAA–Lawson methods substantially outperform Padé

approximants and global approximation methods such as Chebyshev based methods.

Structure-preserving discontinuous Galerkin methods for the Poisson-Nernst-Planck system

Alex Trenam & Tristan Pryer *(University of Bath)*

The Poisson-Nernst-Planck (PNP) model of electrodiffusion is a continuum approximation describing the transport of charged particles, which are influenced by each other and the presence of a global electric field. As an example, one could consider the transport of ions in an electrolyte or the evolution of electron and hole densities in semi-conductors.

In its simplest form, the problem is to seek (in some relevant domain with appropriate boundary conditions) the concentrations of positive ρ and negative ν charge carriers and the electric potential ψ, which determines the electric field $\nabla\psi$, satisfying

$$\frac{\partial \rho}{\partial t} = \operatorname{div}\left(\nabla\rho + \rho\nabla\psi\right), \tag{1}$$

$$\frac{\partial \nu}{\partial t} = \operatorname{div}\left(\nabla\nu - \nu\nabla\psi\right), \tag{2}$$

$$-\Delta\psi = \rho - \nu. \tag{3}$$

Given the model's wide range of applications, there is a rich literature of numerical methods for the problem, with a recent particular focus on structure-preserving discretisations. However, the non-linearities in the system present a challenge when designing such methods.

In this talk we present novel discontinuous Galerkin finite element methods for the PNP system, which linearise the problem and unconditionally preserve at the discrete level analogues of important structures inherent to the continuous system: mass conservation, positivity-preservation of charge concentrations, and energy/entropy dissipation laws.

Computing Brascamp-Lieb Constants through the lens of Thompson Geometry

Melanie Weber & Suvrit Sra *(Harvard University)*

In a seminal paper, Brascamp and Lieb (1976) introduced a class of inequalities (*Brascamp-Lieb inequalities*) that generalizes many well-known inequalities, including Hölder's inequality, the sharp Young convolution inequality, and the Loomis-Whitney inequality. As such, the class of Brascamp-Lieb inequalities provides a valuable tool of use to many areas of Mathematics. Furthermore, Brascamp-Lieb inequalities have applications in Machine Learning and Information Theory.

Each Brascamp-Lieb (BL) inequality is characterized by a *BL-datum* $(\mathcal{A}, w)$, consisting of a tuple of linear transformations $\mathcal{A} = \left(A_1, \ldots, A_m\right)$ and a set of exponents $w = \{w_j\}$. Of central importance is the feasibility of the BL-datum, which is characterized by the associated Brascamp-Lieb constant. The computation of this constant is equivalent to solving the following optimization problem over the positive definite matrices ($\mathbb{P}_d$):

$$\min_{X\in\mathbb{P}_d} F(X) := \sum_j w_j \log\det\left(A_j^* X A_j\right) - \log\det(X)\,. \tag{1}$$

In the prior literature, both Euclidean and Riemannian optimization techniques for solving Eq. (1) have been proposed, the latter exploiting the geodesic convexity of the objective. In this talk, we study Picard iterations obtained by iterating a nonlinear map (Weber and Sra 2022)

$$G: \quad X \mapsto \Big(\sum_j w_j A_j \big(A_j^* X A_j\big)^{-1} A_j^*\Big)^{-1}. \tag{2}$$

The simplicity of the map (2) makes the fixed-point approach particularly attractive, since it avoids expensive Riemannian operations such as exponential maps and parallel transports, which are required by standard Riemannian optimization approaches. Indeed, empirically, iterating map (2) exhibits linear convergence. We will present a detailed non-asymptotic convergence analysis of the fixed-point approach, which relies on viewing $\mathbb{P}_d$ as a metric space endowed with the Thompson part metric.

References

[1.] Herm Jan Brascamp and Elliott H Lieb. Best constants in Young's inequality, its converse, and its generalization to more than three functions. *Advances in Mathematics*, 20(2): 151–173, 1976.

[2.] Melanie Weber and Suvrit Sra. Computing Bras camp-Lieb constants through the lens of Thompson Geometry. *arXiv:2208.05013*, 2022.

Generalizing Quasi-Newton Updates to Higher-Order Derivative Tensors

Karl Welzel & Raphael A. Hauser *(University of Oxford)*

At the heart of all quasi-Newton methods is an update rule that enables us to gradually improve the Hessian approximation using the already available gradient evaluations. Theoretical results show that the global performance of optimization algorithms can be improved with higher-order derivatives. This motivates an investigation of generalizations of quasi-Newton update rules to obtain for example third derivatives (which are tensors) from Hessian evaluations. Our generalization is based on the observation that quasi-Newton updates are least-change updates satisfying the secant equation, with different methods using different norms to measure the size of the change. We present a full characterization for least-change updates in weighted Frobenius norms (satisfying an analogue of the secant equation) for derivatives of arbitrary order. Moreover, we establish convergence of the approximations to the true derivative under standard assumptions and explore the quality of the generated approximations in numerical experiments.

Improvement of Mass Conservation in the MINRES Solution of Saddle-Point Systems with Large Right-Hand Sides

Minhui Zhou & Gabriel R. Barrenechea & Jennifer Pestana *(University of Strathclyde)*

We focus on applying the minimum residual method (MINRES) to linear systems arising from finite element discretizations of the Stokes equations, a fundamental viscous flow model. The accuracy of the linear solver MINRES is affected by the size of the norm of the right-hand side (RHS). This is exacerbated by standard MINRES stopping criteria, that do not appropriately capture the size of the RHS. As the magnitude of the forcing term increases, the divergence of the velocity deviates further from zero. It has been proven that this issue cannot be solved due to the homogeneity of a linear system. More precisely, the MINRES algorithm respects the following homogeneity property:

$$\left.\begin{aligned} \mathcal{A}\boldsymbol{x} &= M\boldsymbol{b} \\ \mathcal{A}\tilde{\boldsymbol{x}} &= \boldsymbol{b} \end{aligned}\right\} \rightarrow \boldsymbol{x} = M\tilde{\boldsymbol{x}}.$$

Therefore, we aim to modify MINRES and choose preconditioners so that the resulting algorithm can provide a more accurate solution at an affordable computational cost. This talk shows two potential methods of improvement of the accuracy of MINRES. The first one is to use higher-precision arithmetic within MINRES. The second is to apply a scaled block diagonal preconditioner, which can be equivalently viewed as scaling the Stokes equations. The numerical results show that the accuracy can be significantly improved by applying these two methods.