University of Strathclyde

27th Biennial Conference on Numerical Analysis

27 – 30 June, 2017

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Introduction

Dear Participant,

On behalf of the University of Strathclyde's Numerical Analysis and Scientific Computing Group, it is our pleasure to welcome you to the 27th Biennial Numerical Analysis conference. This is the fifth time the meeting is being held at Strathclyde, continuing the long series of conferences originally hosted in Dundee. We are looking forward to meeting delegates from around the world, with attendees from many different countries across six continents.

Once again, we have been lucky to secure a stellar list of invited speakers who will address us on a variety of topics across all areas of numerical analysis. As well as a selection of specialised minisymposia, we will also have a wide range of contributed talks, so hopefully there is something to suit everyone's interests. Although the meeting is funded almost entirely from the registration fees of the participants, additional financial support for some overseas participants has been provided by the *Dundee Numerical Analysis Fund*, started by Professor Gene Golub from Stanford University in 2007.

As well as attending the scientific sessions, we hope you will also take advantage of the opportunity to renew old friendships and meet new people as part of the communal meals and social programme. We are indebted to the *City of Glasgow* for once again generously sponsoring a wine reception at the City Chambers on Tuesday evening. The building is well worth a visit, featuring a vast range of ornate decoration complete with the largest marble staircase in Western Europe. The conference dinner on Thursday night will be held in another one of Glasgow's historic buildings, the Trades Hall. This was designed and built from 1791–1794 by prominent Scottish architect Robert Adam and, apart from the medieval cathedral, is the oldest building in Glasgow still used for its original purpose.

Thank you for coming, and enjoy the meeting!

Philip Knight
John Mackenzie
Alison Ramage

Conference Organising Committee

Information for participants

- **General**. There will be a registration desk in the foyer of the John Anderson building (building 16 on the campus map, entry on Level 4 from Taylor Street as indicated). The organisers can be contacted there during tea and coffee breaks.
- **Accommodation**. All rooms are in the Campus Village. Check-out time is 10:00 on day of departure. On Friday morning, luggage may be left in room JA3.27.
- **Meals**. Breakfast (Tue-Fri) is available from 07:30 until 09:00 in the Aroma Dining Room in the Lord Todd building (building 26 on the campus map, entry as indicated). The times of lunches and dinners are as indicated in the conference programme. Dinner (Tue-Wed) will also be served in Aroma. Buffet lunches (Tue-Thu) will be served in the Urban Bean Java Cafe (building 18 on the campus map) and (Fri) in the foyer outside JA3.25. Coffee and tea will be provided at the advertised times in the foyer outside JA3.25.
- **Lecture rooms**. These are in the John Anderson building (building 16, enter on Level 4 from Taylor Street). The main auditorium (JA3.25) is down one floor from the main entrance, along with rooms JA3.14 and JA3.17. The additional rooms for parallel sessions are JA4.12 (on the entrance level of the John Anderson building near the registration desk), and JA5.05 and JA5.07 (on level 5 of the John Anderson building).
- **Chairing sessions**. It is hoped that if you are listed as chairing a session, you will be willing to help in this way. Minisymposium organisers should organise chairpeople for their own sessions (including any contributed talks which follow) as appropriate. A break of 5 minutes has been allowed for moving between rooms. Please keep speakers to the timetable!
- **Book displays**. There will be books on display for the duration of the conference in room JA3.26.
- **Reception**. A reception for all participants hosted by Glasgow City Council will be held in the City Chambers on Tuesday 27th June from 20.00 to 21.00. The City Chambers is marked on the campus map: entry is from George Square.
- **Conference dinner**. The conference dinner will be held in the Trades Hall of Glasgow on Thursday 29th June at 20:00 (for 20:30 dinner). The venue is located at 84 Glassford Street, Glasgow G1 1UH, which is 10 minutes walk from the conference venue. The guest speaker will be Professor Ivan Graham, University of Bath.
- **Internet Access**. Complimentary WiFi is available throughout the campus from the 'WifiGuest' network, which should appear on the list of available networks on your portable device. This network uses the same authentication system as 'The Cloud' network found in public places across the UK. You can log in to 'WifiGuest' using existing 'The Cloud' credentials, or set up a new account which you can then use wherever 'The Cloud' is available. More comprehensive internet access is available to eduroam users. Computer terminals will be available from 09:00-17:00 Tuesday-Thursday in room JA5.12 of the John Anderson Building. If you require access to a fixed terminal, please contact the organisers to obtain a username/password.
- **Bar**. There is a bar in the Lord Todd building (building 26) next to the dining room.
- **Sports facilities**. Conference delegates can use the University sports facilities (building 3) by obtaining a card from the Student Village Office. The cost of the facilities varies.

Invited Speakers

Donald Estep	Colorado State University	donald.estep@colostate.edu
Philip Gill	UC San Diego	pgill@ucsd.edu
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Christian Lubich	Universität Tübingen	lubich@na.uni-tuebingen.de
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Gerlind Plonka-Hoch	Universität Göttingen	plonka@math.uni-goettingen.de
Valeria Simoncini	Università di Bologna	valeria.simoncini@unibo.it
Andrew Stuart	Caltech	astuart@caltech.edu
Endre Süli	University of Oxford	endre.suli@maths.ox.ac.uk
Françoise Tisseur	University of Manchester	francoise.tisseur@manchester.ac.uk
Anna-Karin Tornberg	KTH Stockholm	akto@kth.se

Abstracts of Invited Talks

A new approach to stochastic inverse problems for scientific inference

Donald Estep *(Colorado State University)* & Troy Butler *(University of Colorado Denver)*

The stochastic inverse problem for determining parameter values in a physics model from observational data on the output of the model forms the core of scientific inference and engineering design. We describe a recently developed formulation and solution method for stochastic inverse problems that is based on measure theory and a generalization of a contour map. In addition to a complete analytic and numerical theory, advantages of this approach include avoiding the introduction of ad hoc statistics models, unverifiable assumptions, and alterations of the model like regularization. We present a high-dimensional application to determination of parameter fields in storm surge models. We conclude with recent work on defining a notion of condition for stochastic inverse problems and the use in designing sets of optimal observable quantities.

On the contributions of Roger Fletcher and Michael Powell to numerical optimization

Philip E. Gill *(University of California San Diego)*

Very few individuals can be credited with starting a new area of research. Even fewer have repeated this feat over the course of their research careers. Nevertheless, these honors apply to Roger Fletcher and Michael Powell, who made seminal and groundbreaking contributions to many aspects of numerical linear algebra, approximation theory and optimization. In particular, they were jointly responsible for launching the field of nonlinear optimization through the publication of their 1962 paper on what is now known as the DFP algorithm for unconstrained optimization. Numerical optimization continues to have a substantial impact on our everyday lives through its widespread application to problems in engineering and science, as well as its burgeoning use within the area of machine learning and data science. In this talk, I will focus on some of Roger and Mike's contributions to nonlinearly constrained optimization and give some examples of how their work is still relevant in the formulation and analysis of modern optimization methods.

Spectral graph clustering with motifs and higher-order structures

David Gleich *(Purdue University)*

Spectral clustering is a well-known method to divide a graph or network into coherent clusters based on the eigenvectors of a matrix. When the quality of a cluster is measured using the conductance metric, there is a specific sweep-cut procedure that transforms an eigenvector into a cluster that satisfies an approximation guarantee with respect to the best possible cluster. This guarantee is known as the Cheeger inequality and it holds for undirected graphs. We'll discuss a new generalization of the Cheeger inequality to higher-order structures in networks including network motifs such as triangles. The resulting procedure is easy and simple to implement and seamlessly generalizes spectral clustering to directed, signed, and many other types of complex networks. In particular, our generalization allows us to re-use the large history of ideas and research on spectral clustering including eigenvalue solvers and local. We will illustrate the types of clusters or communities found by our new method in a variety of real-world networks such as biological, neuroscience, ecological, transportation, and social networks.

Algorithmic Adaptations to Extreme Scale Computing

David E. Keyes *(KAUST)*

Algorithmic adaptations to use next-generation computers close to their potential are underway. Instead of squeezing out flops the traditional goal of algorithmic optimality, which once served as a reasonable proxy for all associated costs algorithms must now squeeze synchronizations, memory, and data transfers, while extra flops on locally cached data represent only small costs in time and energy. After decades of programming model stability with bulk synchronous processing, new programming models and new algorithmic capabilities (to make forays into, e.g., data assimilation, inverse problems, and uncertainty quantification) must be co-designed with the hardware. We briefly recap the architectural constraints and application opportunities. We then concentrate on two types of tasks each of which occupies a large portion of all scientific computing cycles: large dense symmetric/Hermitian linear systems (covariances, Hamiltonians, Hessians, Schur complements) and large sparse Poisson/Helmholtz systems (solids, fluids, electromag-

netism, radiation diffusion, gravitation). We examine progress in porting solvers for these tasks to the hybrid distributed-shared programming environment, including the GPU and the MIC architectures that make up the cores of the top scientific computers "on the floor" and "on the books".

Dynamical low-rank approximation

Christian Lubich *(University of Tübingen)*

This talk reviews differential equations on manifolds of low-rank matrices or tensors or tensor tree networks. They serve to approximate, in a data-compressed format, large time-dependent matrices and tensors that are either given explicitly via their increments or are unknown solutions of high-dimensional differential equations, such as multi-particle time-dependent Schrödinger equations. Recently developed numerical time integrators are based on splitting the projector onto the tangent space of the low-rank manifold at the current approximation. In contrast to all standard integrators, these projector-splitting methods are robust with respect to the unavoidable presence of small singular values in the low-rank approximation. This robustness relies on geometric properties of the low-rank manifolds.

The talk is based on work done intermittently over the last decade with Othmar Koch, Bart Vandereycken, Ivan Oseledets, Emil Kieri and Hanna Walach.

Trefftz finite element methods

Ilaria Perugia *(University of Vienna)*

Over the last years, finite element methods based on operator-adapted approximating spaces have been developed in order to better reproduce physical properties of the analytical solutions, and to enhance stability and approximation properties. They are based on incorporating a priori knowledge about the problem into the local approximating spaces, by using trial and/or test spaces locally spanned by functions belonging to the kernel of the differential operator (Trefftz spaces). These methods are particularly popular for wave problems in frequency domain. Here, the use of oscillating basis functions allows to improve the accuracy vs. computational cost, with respect to standard polynomial finite element methods, and breaks the strong requirements on number of degrees of freedom per wavelength to ensure stability.

In this talk, the basic principles of Trefftz finite element methods for time-harmonic wave problems will be presented. Trefftz methods differ from each other by the way interelement continuity conditions are imposed. We will focus on discontinuous Galerkin approaches, where the approximating spaces are made of completely discontinuous Trefftz spaces, and on the recent virtual element framework, which allows for the construction of Trefftz-enriched continuous spaces on general polytopic meshes.

Deterministic Sparse FFT Algorithms

Gerlind Plonka & Katrin Wannenwetsch *(University of Göttingen)*

We consider some ideas to improve the well-known (inverse) FFT algorithm to compute a complex vector $\mathbf{x}$ of length N from its Fourier transformed data. It is known that the FFT of length N needs $\mathcal{O}(N \log N)$ arithmetical operations. However, if the resulting vector $\mathbf{x}$ is a priori known to be sparse, i.e., contains only a small number of non-zero components, the question arises, whether we can do this computation in an even faster way. In recent years, different sublinear algorithms for the sparse FFT have been proposed, most of them are randomized. We want to concentrate on deterministic sparse FFT algorithms. The talk is based on joint work with Katrin Wannenwetsch, Annie Cuyt and Wen-Shin Lee.

References

[1] G. Plonka and K. Wannenwetsch, A deterministic sparse FFT algorithm for vectors with small support, Numerical Algorithms **71**(4) (2016), 889–905.

[2] G. Plonka and K. Wannenwetsch, A sparse fast Fourier algorithm for real nonnegative vectors, J. Comput. Appl. Math. **321** (2017), 532–539.

[3] G. Plonka, K. Wannenwetsch, A. Cuyt, and W.-S. Lee, Deterministic sparse FFT for non-negative M-sparse vectors, preprint 2017.

Computational methods for large-scale matrix equations: recent advances and applications

Valeria Simoncini *(Università di Bologna)*

Linear matrix equations such as the Lyapunov and Sylvester equations and their generalizations have classically played an important role in the analysis of dy-

namical systems, in control theory and in eigenvalue computation. More recently, matrix equations have emerged as a natural linear algebra framework for the discretized version of (systems of) partial differential equations, and new challenges have arisen.

Several well established and robust algorithms exist for the solution of small dimensional linear matrix equations, whereas only in the past decades major steps ahead have been made in the large scale case.

In this talk we review some of the key methodologies behind these new algorithms, highlighting both the theoretical and computational aspects. Moreover, we will discuss recent strategies for the numerical solution of more advanced equations, such as multiterm linear matrix equations and bilinear systems of equations, which are currently attracting great interest due to their occurrence in new application models.

Large Graph Limits of Classification Algorithms

A. M. Stuart *(Caltech)*

Many problems in machine learning require the classification of high dimensional data. One methodology to approach such problems is to construct a graph whose nodes are identified with data points, with edges weighted according to some measure of affinity between the data points. Algorithms such as spectral clustering, probit classification and the Bayesian level set method can all be applied in this setting. The goal of the talk is to describe these algorithms for classification, and analyze them in the limit of large data sets. Doing so leads to interesting problems in the calculus of variations, in stochastic partial differential equations and in Monte Carlo Markov Chain, all of which will be highlighted in the talk. These limiting problems give insight into the structure of the classification problem, and algorithms for it.

Collaboration with Matt Dunlop (Caltech), Dejan Slepcev (CMU), and Matt Thorpe (CMU).

Finite element approximation of implicitly constituted fluid flow models

Endre Süli *(University of Oxford)*

Classical models describing the motion of Newtonian fluids, such as water, rely on the assumption that the Cauchy stress is a linear function of the symmetric part of the velocity gradient of the fluid. This assumption leads to the Navier–Stokes equations. It is known however that the framework of classical continuum mechanics, built upon an explicit constitutive equation for the Cauchy stress, is too narrow to describe inelastic behavior of solid-like materials or viscoelastic properties of materials. Our starting point in this work is therefore a generalization of the classical framework of continuum mechanics, called the *implicit constitutive theory*, which was proposed recently in a series of papers by Rajagopal. The underlying principle of the implicit constitutive theory in the context of viscous flows is the following: instead of demanding that the Cauchy stress is an explicit (and, in particular, linear) function of the symmetric part of the velocity gradient, one may allow a nonlinear, implicit and not necessarily continuous relationship between these quantities. The resulting general theory therefore admits non-Newtonian fluid flow models with implicit and possibly discontinuous power-law-like rheology.

We develop the analysis of finite element approximations of implicit power-law-like models for viscous incompressible fluids. The Cauchy stress and the symmetric part of the velocity gradient in the class of models under consideration are related by a, possibly multi-valued, maximal monotone graph. Using a variety of weak compactness techniques, including Chacon's biting lemma, we show that a subsequence of the sequence of finite element solutions converges to a weak solution of the problem as the discretization parameter, measuring the granularity of the finite element triangulation, tends to zero. A key new technical tool in our analysis is a finite element counterpart of the Acerbi–Fusco Lipschitz truncation of Sobolev functions.

The talk is based on a series of recent papers with Lars Diening (Bielefeld) and Christian Kreuzer (Dortmund), and ongoing research with Tabea Tscherpel (Oxford).

Exploiting Tropical Algebra in Numerical Linear Algebra

Françoise Tisseur *(University of Manchester)*

The objective of this talk is to explore applications of tropical algebra to numerical linear algebra. The *tropical semiring* consists of the extended reals $\overline{\mathbb{R}} = \mathbb{R} \cup \{-\infty\}$ along with two binary operations, an addition and a multiplication, defined by, $a \oplus b = \max(a, b)$ and $a \otimes b = a + b$ for all $a, b \in \overline{\mathbb{R}}$, where $-\infty$ and 0 are the additive and multiplicative identities, respectively. Any semiring equipped with min or max as the addition operation is known as tropical. The

link between the usual and tropical algebras is provided by a *valuation*, a typical valuation for complex numbers being $x \in \mathbb{C} \mapsto \mathcal{V}(x) = \log|x| \in \overline{\mathbb{R}}$, where by convention $\log 0 = -\infty$. Note that for $x, y \in \mathbb{C}$, $\mathcal{V}(xy) = \mathcal{V}(x) + \mathcal{V}(y)$, and when $|x| \gg |y|$ or $|x| \ll |y|$ then $\mathcal{V}(x+y) \approx \max\{\mathcal{V}(x), \mathcal{V}(y)\}$. This suggests using the operations max and plus in place of the classical addition and multiplication once we have applied the map $\mathcal{V}$.

There are analogues of roots of polynomials, eigenvalues and singular values of matrices, and matrix factorizations in the tropical setting, and when combined with a valuation map these analogues offer order of magnitude approximations to roots of polynomials, eigenvalues and singular values, and factorizations of matrices in the usual algebra. What makes tropical algebra a useful tool for numerical linear algebra is that these tropical analogues are usually cheaper to compute than those in the conventional algebra. They can then be used in the design of preprocessing steps to improve the numerical behaviour of algorithms (convergence, stability, ...). In this talk we concentrate on the use of tropical algebra

1. to construct a new incomplete LU preconditioner that is usually almost as cheap to compute as ILU(k) but has properties similar to the more effective but more expensive to compute threshold incomplete LU preconditioner, and

2. to improve the numerical stability of polynomial eigensolvers of arbitrary degree, and to design a numerically stable quadratic eigensolver.

This is joint work with James Hook, Marc Van Barel, and Laurence Grammont.

Accurate evaluation of layer potentials in integral equations

Anna-Karin Tornberg *(KTH Royal Institute of Technology, Stockholm)*

Near singularities arise from Green's functions as single and double layer potentials are evaluated close to boundaries and interfaces in an integral equation based method. The quadrature error for this integral evaluation increases exponentially as the boundary is approached if a regular quadrature rule is used.

Starting in 2D, we present very precise estimates for the quadrature errors, that are derived using a technique based on contour integration and calculus of residues. These estimates can determine when the regular quadrature fails to keep the error below a set tolerance.

Quadrature by expansion (QBX) is a new specialized quadrature method that can evaluate nearly singular integrals very accurately. There are however several parameters to choose for this method. Similar to the layer potential, estimates can be derived also for the error in the coefficients of the expansion underlying QBX, and this can be used to create an adaptive QBX method that self-selects parameters, given an error tolerance. The performance of this method is discussed for Laplace and Helmholtz equations in 2D.

We also discuss QBX in three dimensions for Stokes flow. We show how to extend the error estimates to integrals over surfaces in three dimensions. We discuss a QBX method for solid ellipsoids and rigid walls, where precomputations are made using geometric symmetries to reduce computations and storage. Finally, we discuss the development of a target-specific QBX method for deformable drops, where all computations must be made on the fly.

Minisymposia abstracts

Minisymposium M1

Numerical Methods for Nonlocal Problems
Organisers
Mihály Kovács and Bangti Jin

Space Fractional PDEs on bounded domains

Boris Baeumer & Mihály Kovács & Harish Sankaranarayanan *(University of Otago)*

We identify various boundary conditions for spatially fractional PDEs and the associated stochastic processes governed by them.

Discretisations of fractional powers of the Laplacian in bounded domains

Félix del Teso & Nicole Cusimano *(BCAM)* & Luca Gerardo-Giorda *(BCAM)* & Gianni Pagnini *(BCAM)*

The fractional Laplacian is a differential operator of non-integer order that has been extensively studied in the last few decades and is naturally defined on the whole $\mathbb{R}^N$. As many other fractional order derivatives and integrals, this operator has often been used to model transport processes which generalise classical Brownian motion. However, many physical problems of interest are defined in bounded domains and the use of the fractional Laplacian as a modelling tool in this context poses the challenge of providing a meaningful interpretation of the operator in these settings. Following the heat semi-group formalism, we introduce a family of operators which are boundary conditions dependent and discuss a suitable approach for their numerical discretisation by combining a quadrature rule of integration with the finite element method. This approach will not only allow for a meaningful interpretation of fractional powers of an operator in bounded settings but will also provide a flexible strategy for the computation of their value on multi-dimensional (possibly irregular) domains, and a convenient framework for the solution of the fractional Poisson equation and the corresponding parabolic problem.

Numerical methods for nonlinear nonlocal PDEs and their convergence analysis

Espen R. Jakobsen *(Norwegian University of Science and Technology (NTNU))*

In this talk we focus on numerical methods for nonlocal diffusion equations

$$u_t - \mathcal{L}\varphi(u) = g,$$

or convection-diffusion equations

$$v_t + \nabla \cdot f(v) - \mathcal{L}\varphi(v) = g.$$

Here $\mathcal{L}$ is a nonlocal diffusion operator and the generator of a Levy process. Our admissible class of operators is very large and includes e.g. the fractional Laplacian $(-\Delta)^{\frac{\alpha}{2}}$ for $\alpha \in (0, 2)$. In the first part of the talk we briefly mention several different numerical methods that we have proposed and analyzed in recent years: Difference-quadrature methods, discontinuous Galerkin methods, and spectral vanishing viscosity methods. Then in the main part of the talk, we explain the latest results on monotone difference-quadrature approximations for nonlinear diffusion equations of porous medium type. These results include well-posedness, a priori estimates, and convergence for the schemes. The convergence result follows from a compactness argument, stability results, and recent uniqueness results for the limit equation.

The results of the second part of the talk are joint work with Felix del Teso and Jørgen Endal.

Time stepping schemes for fractional diffusion

Bangti Jin *(University College London)*

Fractional diffusion arises in a number of practical applications, e.g., flow in heterogeneous media, thermal diffusion in fractal domains. One mathematical model to describe the physical process is the subdiffusion equation, which involves a Caputo fractional derivative in time. The nonlocality of the fractional derivative leads to limited smoothing property, which poses a significant challenge in the design and analysis of robust numerical schemes. In this talk, I shall discuss some recent progress, e.g., the convolution quadrature and L1 scheme, for discretizing such equations in time. Error estimates and qualitative properties will be discussed.

Numerical solution of fractional order elliptic equations with spatial white noise

Mihály Kovács *(Chalmers/Gothenburg University)* & David Bolin *(Chalmers/Gothenburg University)* & Kristin Kirchner *(Chalmers/Gothenburg University)*

We consider a linear elliptic equation in a bounded spatial domain with additive spatial white noise perturbation where the differential operator is non-local; namely, it is given by the fractional power of an integer order differential operator. These equations play an important role in spatial statistics due to their relation to Gaussian Matérn fields. We use a standard continuous finite element discretization in space together with a quadrature to approximate an integral representation of the fractional power of the inverse of the differential operator. This leads to an algorithm where the solution of several elliptic problems are required. However, these are integer order and hence easily solvable by standard finite element solvers. We analyse the strong rate of convergence of the method in space dimensions 1,2 and 3.

Convergence of finite element solutions of stochastic time-fractional PDEs driven by a space-time white noise

Buyang Li *(The Hong Kong Polytechnic University)*

The stochastic time-fractional equation

$$\partial_t \psi - \Delta \partial_t^{1-\alpha} \psi = f + \dot{W},$$

with space-time white noise $\dot{W}$, is discretized in time by a backward-Euler convolution quadrature, discretized in space by truncating a series representation of the space-time white noise. The truncated problem is solved by the Galerkin finite element method. For the resulting fully discrete numerical scheme, we prove the convergence

$$\mathbb{E}\|\psi(\cdot,t_n) - \psi_n^{(h)}\|_{L^2(\mathcal{O})} =$$

$$\begin{cases} O\big(\tau^{\frac{1}{2}-\frac{\alpha d}{4}} + \ell_h h^{\frac{1}{\alpha}-\frac{d}{2}}\big) & \text{if } \alpha \in \big[\frac{1}{2}, \frac{2}{d}\big), \\ O\big(\tau^{\frac{1}{2}-\frac{\alpha d}{4}} + h^{2-\frac{d}{2}}\big) & \text{if } \alpha \in \big(0, \frac{1}{2}\big), \end{cases}$$

which is sharp up to a logarithmic factor $\ell_h = \ln(2 + 1/h)$, in general d-dimensional spatial domains with nonsmooth data $\psi_0 \in L^2(\mathcal{O})$ and $f \in L^p(0,T;L^2(\mathcal{O}))$, $p > \frac{4}{2+\alpha d}$, $d = 1, 2, 3$.

The main contributions of this paper are the following.

(1) Sharper-order spatial convergence is proved in the case $\alpha \in (1,2)$ and $d = 1$.
(2) The error estimates are extended to $\alpha \in (0, \frac{2}{d})$ and multi-dimensional domains.
(3) An interesting phenomenon is found: the spatial order of convergence $\frac{1}{\alpha} - \frac{d}{2}$ increases to $2 - \frac{d}{2}$ as α decreases to $\frac{1}{2}$, and stays at this order when α further decreases.
(4) Less regularity assumption on f: the error estimates in the literature all rely on certain regularity of $\frac{\partial f}{\partial t}$. We relax such conditions to certain integrability of f to match the convergence rate of the stochastic problem. Consequently, the source f does not need to be continuous in time.

Fast and oblivious convolution quadrature for wave problems

María López-Fernández & Lehel Banjai, Achim Schädle *(Sapienza University of Rome)*

The use of time-domain boundary integral equations has proved very effective and efficient for three dimensional acoustic and electromagnetic wave equations. In even dimensions and when some dissipation is present, time-domain boundary equations contain an infinite memory tail. Due to this, computation for longer times becomes exceedingly expensive. We will show how fast and oblivious convolution quadrature, initially designed for parabolic problems, can be used to significantly reduce both the cost and the memory requirements of computing this tail. We analyse Runge-Kutta based convolution quadrature and conclude with some numerical experiments.

Numerical method for a time-space fractional Fokker Planck equation

Ercília Sousa *(University of Coimbra)*

We consider a time-space fractional Fokker-Planck equation with a force and diffusion depending on space and time. In the case of time dependent coefficients the time fractional operator that typically appears on the right hand side of the fractional equation can not act in those coefficients and therefore the differential equation can not be simplified using the standard technique of transferring the time fractional operator to the left hand side of the equation. We present a numerical method that takes into consideration the fact that the time fractional operator does not act in the time dependent coefficients. Discussions on the stability and accuracy of the numerical method are included. We also present results that show how the order of convergence of the numerical method depends

on the regularity of the solutions. This talk is based on joint work with Luis Pinto from University of Coimbra.

A graded-mesh finite difference scheme for a time-fractional diffusion equation

Martin Stynes & Eugene O'Riordan & José Luis Gracia *(Beijing Computational Science Research Center)*

A reaction-diffusion problem with a Caputo time derivative of order $\delta \in (0,1)$ is considered. The solution of such a problem is shown in general to have a weak singularity near the initial time $t = 0$, and sharp pointwise bounds on certain derivatives of this solution are derived. A new analysis of a standard finite difference method for the problem is given, taking into account this initial singularity. This analysis encompasses both uniform meshes and meshes that are graded in time, and includes new stability and consistency bounds. The final convergence result shows clearly how the regularity of the solution and the grading of the mesh affect the order of convergence of the difference scheme, so one can choose an optimal mesh grading. Numerical results are presented that confirm the sharpness of the error analysis.

Minisymposium M2

Recent Advances in the Numerical Solution of Large-Scale Inverse Problems

Organiser
Silvia Gazzola

Variational methods for dynamical photoacoustic imaging

Marta M. Betcke & Felix Lucka, Nam Huynh, Ben Cox, Edward Zhang, Bradley Treeby, Paul Beard and Simon Arridge *(University College London)*

In photoacoustic imaging, as in many high resolution modalities, the major bottle neck is the acquisition time of finely spatially sampled data. In particular for imaging of dynamical processes, this results in incomplete data. In this talk we are going to discuss variational methods for photoacoustic imaging and their particular realisation in the framework of k-space pseudo-spectral methods. Our framework is general enough to accommodate different approaches to acceleration such as subsampling or compressed sensing which allow us to collect considerably fewer measurements while maintaining good quality of the reconstruction through suitable regularisation.

Accelerated Stochastic PDHG by Non-Uniform Sampling

Matthias J. Ehrhardt, Antonin Chambolle, Peter Richtárik & Carola-Bibiane Schönlieb *(University of Cambridge)*

A very popular algorithm for image processing and image reconstruction with non-differentiable priors is the primal-dual hybrid gradient (PDHG) algorithm proposed by Chambolle and Pock. In some scenarios it is beneficial to employ a stochastic version of this algorithm where not all of the dual updates are executed simultaneously. In this talk we will discuss extensions to non-uniform parameter choices and non-uniform sampling and show that the algorithm converges linearly for strongly convex problems—even for this generalized setting.

Transpose-free methods for linear inverse problems

Silvia Gazzola & Paolo Novati *(University of Bath)*

This talk introduces and analyses an original class of Krylov subspace methods that provide an efficient alternative to many well-known conjugate-gradient-like Krylov solvers for square nonsymmetric linear systems $Ax = b$ arising from discretisations of inverse ill-posed problems. The main idea underlying the new methods is to consider some rank-deficient approximations of the transpose of the system matrix, obtained by running the (transpose-free) Arnoldi algorithm, and then apply some Krylov solvers to a formally right-preconditioned system of equations. These new methods are particularly meaningful when dealing with large-scale problems, and in those situations when A^T is unavailable, or matrix-vector products with A^T are impractical to compute. Theoretical insight is given, and the results of many numerical tests are presented to show that, in a variety of situations, the new solvers outperform the classical Arnoldi-based or conjugate-gradient-like methods.

A low-rank approach to the solution of weak constraint variational data assimilation prob-

lems

Daniel L. H. Green & Melina A. Freitag *(University of Bath)*

Weak constraint four-dimensional variational data assimilation is an important method for incorporating data (typically observations) into a model. The linearised system arising within the minimisation process can be formulated as a saddle point problem. A disadvantage of this formulation is the large storage requirements involved in the linear system. In this talk, we present a low-rank approach which exploits the structure of the saddle point system using techniques and theory from solving large scale matrix equations. Numerical experiments with the linear advection-diffusion equation, and the non-linear Lorenz-95 model demonstrate the effectiveness of a low-rank Krylov subspace solver when compared to a traditional solver.

The conditioning of variational data assimilation with correlated observation errors

Amos Lawless, Jemima Tabeart, Sarah Dance, Nancy Nichols, Joanne Waller *(University of Reading)* & Stefano Migliorini, Fiona Smith *(Met Office)*

Data assimilation is the process of combining measurements of a dynamical system with a numerical model in order to estimate the state of the system. It is widely used in environmental forecasting as a means of obtaining initial conditions for forecast models. Variational data assimilation (Var) formulates the problem as the minimisation of a weighted non-linear least-squares cost function, in which the fit to the measurements is balanced against the fit to a previous model forecast. These two terms are weighted by matrices describing the correlations of the errors in the forecast and of errors in the observations. In practice an incremental version of Var is implemented, in which a series of linear approximations to the non-linear cost function is minimized using an iterative optimisation algorithm. This is equivalent to an approximate Gauss-Newton method. The rate of convergence of the iteration scheme and the sensitivity of the analysis to perturbations in the data are bounded by the condition number of the optimisation problem.

Until recently most operational weather and ocean forecasting systems assumed that the errors in the observations are uncorrelated. However, in practice this is not always true and as we move to higher resolution observations then it is becoming more important to specify observation error correlations. In this work we look at the effect this has on the conditioning of the minimisation problem. We develop theoretical bounds on the condition number of the problem in the presence of correlated observation errors. We show that the condition number is very dependent on the minimum eigenvalue of the observation error correlation matrix. Results are illustrated numerically in an idealised system, where we find that the behaviour of the condition number as the background and observation correlation length scales change is sensitive to the spatial distribution of observations.

We then present results using the Met Office one-dimensional variational assimilation system, used for preprocessing of satellite observations from the Infrared Atmospheric Sounding Interferometer (IASI) instrument. For this system the observation error correlations are diagnosed from data, but the raw matrices from these diagnostics are highly ill-conditioned and need to be reconditioned before being used operationally. We compare different methods for reconditioning the correlation matrix and examine the effect of these on the convergence rate of the assimilation scheme.

A robust convergent multigrid solver for PDEs with non-smooth coefficients applied to selective segmentation models in 2D and 3D

Mike Roberts & Ke Chen & Klaus Irion *(Liverpool University & Royal Liverpool and Broadgreen University Hospitals NHS Trust)*

In medical imaging selective segmentation of objects in images for identification of abnormalities is incredibly important. It is also important that this segmentation be achieved quickly with minimal input from the user. In this talk I will discuss a fast multigrid solver developed for a class of selective segmentation models in 2D and 3D. One key challenge of the multigrid algorithm is that it does not converge if the underlying smoother is not effective at smoothing out errors. If the iterative scheme derived from a discretised PDE has non-smooth coefficients then we find smoothers to be ineffective and multigrid fails to converge. We have developed a class of non-standard smoothers which tackle the non-smoothness directly and locally to give an effective smoother and a convergent multigrid scheme. The implementation of this allows very quick segmentation of user selected items within an image. Various results will be shown and further problems discussed.

Minisymposium M3

Numerical Methods for Coupled Bulk-Surface Problems
Organisers
John Mackenzie and Anotida Madzvamuse

Numerical preservation of invariant regions for reaction-cross-diffusion systems on evolving surfaces

Massimo Frittelli & Anotida Madzvamuse & Ivonne Sgura & Chandrasekhar Venkataraman *(Università del Salento)*

We propose and analyse a finite element method with mass lumping for the numerical approximation of reaction-cross-diffusion systems (RCDSs) on surfaces in $\mathbb{R}^3$ that evolve under a given velocity field. We provide a fully-discrete method based on the IMEX Euler time discretisation. We prove, under the assumption that the mesh preserves the Delaunay regularity under evolution, a sufficient condition for the existence of invariant regions (i) at the spatially discrete level with no restriction on the mesh size and (ii) at the fully-discrete level under a timestep restriction that depends on the kinetics, only. For the special cases of RCDSs (i) on planar domains and (ii) on stationary surfaces in the absence of cross-diffusion, a theory of invariant regions *at the continuous level* is available in the literature, see [J.Smoller, "Shock waves and reaction-diffusion equations", 1983] and [M. Taylor, "Partial differential equations III", 2010]. Hence, in these special cases our results imply the *preservation* of invariant regions under discretisation. In the most general case of RCDSs on arbitrary evolving surfaces for which, to the best of the authors' knowledge, no invariant region theory at the continuous level is available, our results suggest a research direction in the pure analysis of RCDSs on evolving surfaces. Numerical examples are provided to validate the theoretical findings.

An Adaptive Moving Mesh Method for Geometric Evolutions Laws and Bulk-Surface PDEs

John Mackenzie & Michael Nolan & Christopher Rowlatt *(University of Strathclyde)*

The solution of coupled PDEs on evolving bulk and surface domains pose many challenges. In this talk we begin by considering the adaptive numerical solution of curve-shortening flow with a driving force. An adaptive moving mesh approach is used to distribute the mesh points in the tangential direction. This ensures that the resulting meshes evolve smoothly in time and are well adjusted to resolve areas of high curvature. Experiments will be presented to highlight the improvement in accuracy obtained using the new method in comparison with uniform arc-length mesh distributions. We will also discuss the use of the evolving adaptive curve mesh in the adaptive generation of bulk meshes for the solution of bulk-surface PDEs in time dependent domains. In particular, we develop a conservative arbitrary Lagrangian-Eulerian finite element method for mass-conservative reaction-diffusion systems on evolving domains which model intracellular signalling in cell biology.

Numerical methods for understanding nematode locomotion

Thomas Ranner *(University of Leeds)*

The microscopic roundworm C. elegans has long been an important model organism in many biological areas. In particular in recent years researchers from many different have used C. elegans as a model organism to derive an integrated understanding of undulatory locomotion including fluid dynamics, body mechanics and neuro-dynamics. In this talk, we will discuss a continuum model which accurately captures the worm's body mechanics. Following a careful non-dimensionalisation, the resulting equations are similar to equations for an elastic beam subject to a local length constraint. The non-dimensionalised equation can be discretised by a mixed piecewise linear-piecewise constant finite element method and semi-implicit discretisation in time which results in a linear system of equations to be solved at each time step. Numerical examples demonstrate that a careful writing of the constraint equation adds extra stability and accuracy in the method. Further examples show the efficacy of the method over a wide physically relevant parameter range. Finally, it will be shown that the numerical method can be extended to be used as part of a novel imaging set up which captures C. elegans locomotion in three dimensions for the first time.

A diffuse interface approach to PDEs on networks and bubble clusters

Björn Stinner & Andreas Dedner & Oliver Dunbar *(University of Warwick)*

Soluble surface active agents (surfactants) in multi-phase flow with three or more fluids can be described by coupled bulk and interface advection-diffusion equations. Modelling the multi-phase flow with a Cahn-Hilliard-Navier-Stokes system leads to thin interfacial layers and requires suitable methods for the bulk or interface resident surfactant fields. One key challenge is to correctly recover the conditions in the triple junctions where three or more fluids meet. We will therefore focus on a diffuse interface approach to partial differential equations on evolving bubble clusters and network-like structures. Thanks to smoothing the problem by replacing the interfaces with thin layers standard bulk finite elements can be employed. Mesh adaptation is mandatory to make simulations feasible. Some simulation results will be presented in order to support the theoretical predictions for the method.

Asymptotic limits of models for receptor-ligand dynamics

Chandrasekhar Venkataraman *(University of St Andrews)*

We consider coupled bulk-surface systems of partial differential equations, that arise in models for receptor-ligand interactions. Biological considerations motivate the study of a number of asymptotic limits of the model.

In this talk we develop a mathematical theory for the treatment of the original equations together with certain asymptotic limits. The theoretical results will be supported by computations of the original and reduced problems for which we employ a bulk-surface finite element method.

Experimentally-Driven Mathematics for Particle and Whole Cell Migration

Feng Wei Yang & Anotida Madzvamuse *(University of Sussex)*

Mathematical analysis and modelling are becoming increasingly important in cell biology as they provide a theoretical and computational framework for analysing experimental data, quantitatively and qualitatively, and hence furthering our understanding of dynamic cellular phenomena. However, in order to draw conclusions from the experiment, as well as provide actual measurements to modelling, real world data has to be processed. The advent of high-throughput, high-resolution microscopy and imaging techniques means that a wealth of large data is routinely generated in many laboratories. Due to the sheer magnitude of the data involved manual processing is not suitable, hence fully-automated computer algorithms have to be developed and applied. In this work, we describe novel approaches for automated cell tracking, which involves segmentation and particle tracking. We also illustrate our modelling approach from which we may reconstruct changes in cell morphology and allows us to predict physical quantities that would be otherwise unavailable from experiments. Our model consists of partial differential equations and involves the optimal control of a phase-field formulation of a geometric evolution law for the cell-membrane motion. We present a series of numerical techniques that allows us to obtain computational results in real time, with substantial reductions in computer memory requirements.

Minisymposium M4

Fast spectral methods for fluid dynamics

Organisers

Alex Townsend and Grady Wright

Large-scale tsunami simulations using the discontinuous Galerkin method

Boris Bonev[*], Jan S. Hesthaven[*], Francis X. Giraldo[†] ([*]*Ecole polytechnique fédérale de Lausanne (EPFL),* [†]*Naval Postgraduate School Monterey*)

Discontinuous Galerkin methods have desirable properties, which make them suitable for the computation of wave problems. Being parallelizable and *hp*-adaptive makes them attractive for the simulation of large-scale tsunami propagation. In order to retrieve such a scheme, we formulate the shallow water equations on the spherical shell and apply the discontinuous Galerkin discretization to construct a numerical method which is able to handle the effects of curvature and Coriolis forces naturally. Common challenges in solving the shallow water equations numerically are well-balancedness and wetting/drying. To overcome this, we utilize a method based on a timestep restriction, which guarantees the positivity of the numerical solution. Moreover, we show that our discretization yields a well-balanced numerical scheme. In this talk we will present our method as well as the numerical results, that we have obtained with our implementa-

tion.

Time-domain Bernstein-Bezier DG methods on simplices

Jesse Chan *(Rice University)* & Tim Warburton *(Virginia Tech)*

Time-domain discontinuous Galerkin methods on unstructured tetrahedral meshes allow for both high order accuracy and geometric flexibility. However, in contrast with spectral methods on tensor product elements, computational costs increase rapidly with the order of approximation when using simplicial elements. We address these issues by utilizing properties of Bernstein-Bezier polynomials, and present a GPU-accelerated implementation. For linear wave propagation problems with piecewise constant coefficients and affine elements, this implementation achieves both optimal complexity operator evaluation and high computational performance. Extensions to high order coefficients and curved elements will also be discussed.

Spectral methods for active biological fluid simulations

Alex Townsend *(Cornell University)*

Highly concentrated fluid suspensions of *Bacillus subtilis* exhibit self-sustained turbulent structures, demonstrating that microswimmers can lead to changes in the macro-dynamics of a fluid. Recently, a high-order generalization of the Navier–Stokes equations has been proposed to study these suspensions. In this talk we describe the underlying spectral methods that have allowed for efficient long-time simulations of active biological fluids in confined geometries such as the disk and solid sphere. This is joint work with Jonasz Słomka and Jörn Dunkel.

Bifurcation analysis for timesteppers

Laurette S. Tuckerman *(CNRS, ESPCI Paris, PSL Research University; Sorbonne Université, Univ. Paris Diderot.)*

Spectral methods in tensor product geometries lend themselves to operations which are simultaneously accurate and fast (proportional to the number of points) even in three dimensions. The main use that is made of this property is in time integration, but it can also be used profitably for steady state solving and linear stability analysis. In this talk, we will show how to adapt a time-stepping code so as to calculate steady states and rotating waves via Newton's method and to calculate leading eigenpairs and Floquet multipliers via the Arnoldi method. We will show how this information can be used to understand various hydrodynamic pattern-forming systems, such as convection in cylindrical and spherical geometries

The plunge region in frame-based approximation

Marcus Webb *(KU Leuven)*

We will discuss new results about the plunge region phenomenon in frame-based approximation which until now have only been empirically observed [1].

Frames: A frame is a generalisation of a basis which can be redundant (i.e. linearly dependent). This redundancy provides a wealth of flexibility and enables rapid approximation of classes of functions that cannot be well approximated by commonly used bases. Examples include functions with a singularity, or multivariate functions defined on irregular domains — situations where non-spectral approximations are typically used out of necessity.

The plunge region: On the other hand, the redundancy also leads to extremely ill-conditioned linear systems. Yet, it can be shown that the computation of best approximations in a frame is numerically stable, in spite of the ill-conditioning. Furthermore, several frames of practical interest give rise to linear systems with a particular singular value structure — a plunge region — that can be exploited to achieve fast approximation algorithms [2].

New results: The key conjecture is that the plunge region is small enough to be exploited for many frames of practical interest. This was already well-known for Fourier extensions, but we prove that for many other types of frames involving trigonometric-like bases such as Fourier and Jacobi polynomials, the plunge region is small, showing that the techniques developed by Matthysen and Huybrechs for Fourier extensions can be applied more generally.

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A high-order meshfree method for advection dominated PDEs on surfaces

Grady Wright *(Boise University)*

We present a new high-order semi-Lagrangian method based on radial basis function interpolation for simulating transport on smooth two-dimensional surfaces. The method is meshfree and formulated entirely in Cartesian coordinates, which permits the use of fairly general node distributions on the surface and entirely avoids (artificial) singularities associated surface based coordinates. The semi-Lagrangian framework allows the new method to bypass the use of any stabilization terms (such as hyperviscosity) during time-integration, thus reducing the number of parameters that have to be tuned. Furthermore, it allows for time-steps that are much larger than the CFL condition allows. Numerical results will be presented demonstrating the high-order accuracy of the method. We will also comment on techniques for improving the efficiency of the method, which at present scales quadratically in the number of unknowns per time-step. Finally, we discuss how the method can be extended to advection-reaction-diffusion equations, which is a first step in our plan to develop a high-order accurate solver for Navier-Stokes equations on general smooth surfaces.

Minisymposium M5

Numerical methods for convection-dominated problems

Organisers

Gabriel Barrenechea and Gert Lube

A low-order stabilised finite element method for the Boussinesq problem

Alejandro Allendes[1], **Gabriel R. Barrenechea**[2] & César Naranjo[1]

[1] *(Universidad Técnica Federico Santa María, Chile)*

[2] *(University of Strathclyde)*

A low-order stabilised finite element method is proposed, analysed, and tested numerically for the steady-state Boussinesq problem. The method uses first order piecewise linear elements for velocity and temperature, and piecewise constant elements for the pressure. One of the main features of the method is that it includes a post-processing for the velocity field in such a way that the discrete velocity fed to the temperature and momentum equations is divergence-free. This post-processing, originally proposed in [2], is included in the discrete problem. This aspect is of great importance in the stability analysis. The presence of convection is stabilised by a LPS-like stabilising term in the Navier-Stokes equation. The convection stabilisation in the temperature equation is done in a very generic way, with possibilities including CIP (cf. [3]), or nonlinear edge based diffusion (cf. [2]). Stability and error analyses are carried out. These follow the general lines given in [4], where BDM elements were used to obtain a divergence-free velocity field, and no stabilisation of the convection was used. Finally, a variety of numerical experiments confirm the theoretical findings.

References

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Pressure-robust H(div)-conforming FEM for transient incompressible flow problems

G. Lube & P.W. Schroeder *(NAM, Georg-August University Göttingen)*

The talk considers the analysis and application of H(div)-conforming, exactly divergence-free FEM with upwind stabilization to time-dependent incompressible flow problems. As a proof of concept, for the transient Oseen problem, we prove semi-discrete error estimates for the velocity that holds independently of both, pressure and Reynolds number. Key aspects are the use of the discrete Stokes projection for the error splitting and the treatment of the convective term.

Emphasising the importance of conservation properties, the theoretical results are complemented with numerical simulations of 2D-vortex dynamics (periodic lattice flow, Kevin-Helmholtz instability, and homogeneous decaying turbulence). We will extend the analysis to the nonlinear case following our approach with H1-conforming methods in Schroeder, Lube: *Pressure-robust analysis of divergence-free and conforming FEM for evolutionary incompressible Navier-Stokes flows*, to appear in *J. Numer. Math. (2017).*

Discontinuous Galerkin time stepping schemes applied to inf-sup stable spatial discretisations of evolutionary Navier–Stokes problems

Gunar Matthies & Naveed Ahmed *(Technische Universität Dresden)*

We consider discontinuous Galerkin time stepping schemes applied to the evolutionary Navier–Stokes equations. The spatial discretisation is based on inf-sup stable pairs of finite element spaces for approximation velocity and pressure. In the case of high Reynolds number, local projection stabilisation of the full gradient is applied.

Using ideas given in [1], we derive for the semi-discretisation in space error estimates which are semi-robust in the Reynolds number provided the velocity solution of the Navier–Stokes problems fulfils sufficient higher regularity assumptions.

The unconditional stability of the fully discrete problem will be proven. Furthermore, optimal error estimates for velocity and pressure will be given for the fully discrete problem where ideas from [2] are applied.

The theoretical findings are confirmed by the numerical simulations.

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Error bounds for non inf-sup stable mixed finite elements for the Navier-Stokes equations with local projection stabilization

Julia Novo *(Universidad Autónoma de Madrid)* & Javier de Frutos, Bosco García-Archilla, Volker John

We consider non inf-sup stable mixed finite elements to approach the evolutionary Navier-Stokes equations. Our aim is to get error bounds with constants independent on inverse powers of the viscosity parameter although depending on the viscosity through norms of the theoretical solution. Different approaches are considered. A method with a general local projection stabilization for the pressure and a global grad-div term is analyzed. For this method we get analogous bounds to those obtained in [2] for inf-sup stable elements. As in [1] error bounds for a primitive in time of the pressure are proved. A second method with local projection stabilization both for the pressure and the grad-div term is considered. In this case our approach is based on the so called term-by-term stabilization method (see [2]). Finally, a method with local projection stabilization for the gradient and for the pressure also based on term-by-term stabilization is considered. For the first two methods error bounds of size $O(h^s)$, h being the mesh diameter, for a solution $(u,p) \in H^{s+1}(\Omega)^d \times H^s(\Omega)$ are obtained while for the last one bounds of order $O(h^{s+1/2})$ for $(u,p) \in H^{s+1}(\Omega)^d \times H^{s+1}(\Omega)$ can be proved.

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Multiscale Hybrid Mixed Method for elliptic Problems

Rodolfo Araya[1], **Diego Paredes**[2] & Frédéric Valentin[3]
[1] *(Universidad de Concepción)*
[2] *(Pontificia Universidad Católica de Valparaíso)*
[3] *(Laboratório Nacional de Computação Científica)*

A family of finite element methods, named Multiscale Hybrid-Mixed method (or MHM for short), aims to solve reactive-advective dominated problems with multiscale coefficients on coarse meshes. The under-

lying upscaling procedure transfers to the basis functions the responsibility of achieving high orders of accuracy. The upscaling is built inside the general framework of hybridization, in which the continuity of the solution is relaxed a priori and imposed weakly through the action of Lagrange multipliers. This characterizes the unknowns as the solutions of local problems with Robin boundary conditions driven by the multipliers. Such local problems are independent of one another, yielding a process naturally shaped for parallelization and adaptivity. Moreover, the multiscale decomposition indicates a new adaptive algorithm to set up local spaces defined using a face-based a posteriori error estimator. Interestingly, it also embeds a postprocessing of the dual variable (flux) which preserves local conservation properties of the exact solution. Extensive numerical validations assess the claimed optimal rates of convergence, the robustness of the method with respect to the model's coefficients, and the adaptivity algorithm.

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A non-linear Petrov-Galerkin method for convection-dominated problems

Sarah Roggendorf[1], Paul Houston[1], Ignacio Muga[2] & Kristoffer G. van der Zee[1] *(1: University of Nottingham; 2: Pontificia Universidad Católica de Valparaíso, Chile)*

If sharp features such as interior or boundary layers are present in the solution of a PDE, the standard Galerkin approach based on a weak formulation in the Hilbert space H^1 frequently leads to highly oscillatory numerical approximations and thus has to be supplemented by suitable stabilisation techniques.

The idea we are pursuing is to consider the approximation problem as a residual minimisation problem in L^p-type Sobolev spaces, cf., [1], with $1 < p < \infty$. We then apply a non-standard, non-linear Petrov-Galerkin discretisation, proposed in [2], that is applicable to reflexive Banach spaces such that the space itself and its dual are strictly convex. Similar to discontinuous Petrov-Galerkin methods [3], this method is based on employing optimal test functions. Replacing the intractable optimal test space by a tractable approximation gives rise to a non-linear inexact mixed method for which optimal a priori estimates hold. For the convection-diffusion equation, this yields a generalization of the approach described in [4] from the L^2-setting to the L^p-setting.

A key advantage of considering a more general Banach space setting is that the oscillations in the numerical approximation vanish as p tends to 1, as we will demonstrate using a few simple numerical examples.

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Error analysis of a variational multiscale stabilization for convection-dominated diffusion equations in 2d

Mira Schedensack & Guanglian Li & Daniel Peterseim *(Univeristät Augsburg)*

This talk formulates a stabilized quasi-optimal Petrov-Galerkin method for singularly perturbed convection-diffusion problems based on the variational multiscale method. The stabilization is of Petrov-Galerkin type with a standard finite element trial space and a

problem-dependent test space based on precomputed fine-scale correctors. The exponential decay of these correctors and their localisation to local patch problems, which depend on the direction of the velocity field and the singular perturbation parameter, is rigorously justified. Under moderate assumptions, this stabilization guarantees stability and quasi-optimal rate of convergence for arbitrary mesh Péclet numbers on fairly coarse meshes at the cost of additional inter-element communication.

Minisymposium M6

Preconditioning
Organisers
Michael Wathen and Jennifer Pestana

Preconditioners for Two-Phase Incompressible Navier–Stokes Flow

Niall Bootland *(University of Oxford)* & Andy Wathen *(University of Oxford)* & Chris Kees *(US Army Coastal and Hydraulics Laboratory)*

Two-phase flows arise in many coastal and hydraulic engineering applications such as the study of coastal waves, dam breaking scenarios, and the design of coastal structures. However, modelling two-phase incompressible flow with a level set formulation results in a variable coefficient Navier–Stokes system that is challenging to solve computationally. Here we consider preconditioners for such systems, looking to adapt efficient preconditioners for single-phase flows. In particular we consider systems arising from the application of finite element methodology and preconditioners based on approximate block factorisation. A crucial ingredient is a good approximation to the Schur complement which can be computed efficiently. To do this, we develop two-phase variants of the pressure convection–diffusion (PCD) and least-squares commutator (LSC) preconditioners.

Field-Of-Values analysis of preconditioned Rayleigh-Bénard convection problems

Giorgio Bornia & Eugenio Aulisa, Victoria Howle, Guoyi Ke *(Texas Tech University)*

In this work we use the notion of field-of-values (FOV) equivalence of matrices to analyze block preconditioners for fixed-point linearizations of the Rayleigh-Bénard convection problem. Finite element discretizations with inf-sup stable velocity-pressure spaces are considered. Sufficient conditions on the model nondimensional parameters are given in order to determine certain notions of equivalence between a class of triangular block preconditioners and the system matrix. Then, some specific preconditioners are considered and their norm- or FOV-equivalence to the system matrix is shown under suitable conditions. Numerical results show that the convergence of the Generalized Minimal Residual method is independent of the mesh size. The performance of the different preconditioners in terms of computational time is also studied.

Circulant preconditioners for systems defined by functions of Toeplitz matrices

Sean Hon *(University of Oxford)*

We propose several circulant preconditioners for the systems defined by functions of Toeplitz matrices, namely $h(A_n)x = b$, where A_n is the Toeplitz matrix generated by certain functions defined on $[-\pi, \pi]$ and $h(x)$ is an analytic function such as e^x, $\sin x$ or $\cos x$. In this talk, we show that $h(c(A_n))$, where $c(A_n)$ is the optimal circulant preconditioner for A_n, can be an effective preconditioner for $h(A_n)$, provided that some conditions are fulfilled. In particular, we show that the eigenvalues of the preconditioned matrix are clustered at ± 1. Hence, accelerated convergence rate of Krylov subspace methods can be expected. Numerical examples are given to support our theoretical results.

Calderón preconditioning for electromagnetic scattering of dielectric objects

Antigoni Kleanthous, Timo Betcke, David Hewett *(UCL)*

In recent years Calderón preconditioning has become a popular strategy to speed up the iterative solution of electromagnetic scattering problems. In this talk we discuss the application of Calderón preconditioners to dielectric scattering problems. We will derive the formulation, discuss its properties, and demonstrate its implementation in the boundary element library BEM++. An application of particular interest to us is the investigation of light scattering properties of ice crystals. We will briefly introduce this problem and demonstrate first examples of applying Calderón

preconditioners to ice crystal scattering problems.

Multipreconditioned GMRES for Shifted Systems

Scott Ladenheim & Tania Bakhos, Peter Kitanidis, Arvind Saibaba, Daniel B. Syzld *(University of Manchester)*

We propose using the multipreconditioned GMRES method for the solution of shifted linear systems with multiple shift-and-invert preconditioners. The multipreconditioned algorithm builds a larger search space by applying each preconditioner to all search directions and computes the minimum norm solution over this larger space. For shift-and-invert preconditioners, the size of the search space grows linearly allowing for a selective and more efficient variant of the algorithm to be implemented. Numerical results from applications in hydraulic tomography and matrix function computations are presented to illustrate the effectiveness of the approach.

Refined saddle-point preconditioners for discretized Stokes problems

Jennifer Pestana, John Pearson & David Silvester *(University of Strathclyde)*

Discretization of the incompressible Stokes equations by stable or stabilized mixed finite elements typically leads to a saddle point system with coefficient matrix

$$\mathcal{A} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix},$$

with $A \in \mathbb{R}^{n\times n}$ symmetric positive definite (SPD), $B \in \mathbb{R}^{m\times n}$, $m < n$, and $C \in \mathbb{R}^{m\times m}$ symmetric positive semidefinite.

When $\mathcal{A}$ is large and sparse, the linear system is often solved by preconditioned MINRES with block diagonal preconditioner

$$\mathcal{P} = \begin{bmatrix} \hat{A} & \\ & \hat{Q} \end{bmatrix},$$

where $\hat{A} \in \mathbb{R}^{n\times n}$ is an SPD approximation of A and $\hat{Q}$ is an SPD approximation of the pressure mass matrix. In this talk we discuss the implications of scaling the (2,2) block of $\mathcal{P}$ by a parameter $\alpha > 0$. In particular, by carefully characterizing the eigenvalues of the preconditioned matrix, and tying these to the convergence of MINRES, we give guidance on the optimal choice of α. Numerical experiments verify our results.

Optimal solvers for linear systems with stochastic PDE origins 'Balanced black-box stopping test'

Pranjal & D. Silvester *(University of Manchester)*

This talk discusses the design and implementation of efficient solution algorithms for symmetric and non-symmetric linear systems arising from FEM approximation of stochastic diffusion and stochastic convection-diffusion problems. The novel feature of our preconditioned MINRES, GMRES, and BICGSTAB(ℓ) solvers is the incorporation of error control in the 'natural' norm in combination with a reliable and efficient a posteriori estimator for the PDE approximation error. This leads to a robust and optimally efficient black-box stopping criterion: the iteration is terminated as soon as the algebraic error is insignificant compared to the approximation error. Our algorithms are optimal in the sense that they result in the savings of unnecessary computations. Also, using the black-box stopping test and a 'good' preconditioner, the suboptimal Krylov solvers like BICGSTAB(ℓ) etc., for which currently little convergence theory exists can be stopped optimally.

Iterative solvers for Q-tensor models of nematic liquid crystals

Alison Ramage *(University of Strathclyde)*

Liquid crystal displays are ubiquitous in modern life, being used extensively in monitors, televisions, gaming devices, watches, telephones etc. Associated mathematical models feature characteristic length and time scales varying by many orders of magnitude, and provide difficult numerical challenges for those trying to simulate real-life dynamic situations. The resulting linear algebra sub-problems frequently involve saddle-point (indefinite) coefficient matrices, which typically arise from the interaction of the liquid crystal material with an applied electric or magnetic field. The efficient solution of these linear systems is of crucial importance for the overall effectiveness of the algorithms used. In this talk, we will discuss preconditioned iterative methods appropriate for solving the coupled set of six partial differential equations which arise from an adaptive finite element Q-tensor based

model of nematic liquid crystal cells.

Solving saddle point systems using short-term recurrences

Tyrone Rees *(STFC Rutherford Appleton Laboratory)*

The need to solve a symmetric, yet indefinite, linear system of the form

$$\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f \\ g \end{pmatrix}$$

arises in practical applications as diverse as weighted least-squares, fluid dynamics, constrained optimization, electronic circuit simulation, and many others. Often the scale of the problem is such that direct methods cannot be used, and we must turn to iterative methods.

The iterative methods that have proved most successful are Krylov subspace methods, and of these Conjugate Gradients (CG) and the Minimal Residual method (MINRES) are particularly attractive, as both methods have the property that the next iterate can be found using only the last few iterates, and they minimize *something* over the entire Krylov subspace.

Conventional wisdom is that CG is not applicable to saddle point problems (since CG can only be applied to a symmetric positive definite system), and MINRES must be applied with a symmetric positive definite preconditioner. However, there are some relatively well known examples that defy this logic. For example, Gould, Hribar and Nocedal showed that, under certain conditions, you can use an (indefinite) constraint preconditioner with CG to solve saddle point systems. Another example was given by Bramble and Pasciak, who described a block lower-triangular preconditioner that can be applied with CG (in a non-standard inner product) to solve saddle point systems.

In this talk I will give some further examples where we can guarantee that CG can be applied to an indefinite problem, or where MINRES can be applied despite not having a symmetric positive definite preconditioner. Such results allow us to employ more powerful preconditioners with these ideal methods, enabling us with the potential to solve larger and more challenging systems.

Two-Stage Preconditioners for Reservoir Simulation

Thomas Roy & Andy Wathen *(University of Oxford)*

Oil and gas reservoir simulation entails solving systems of coupled nonlinear PDEs describing the flow of fluids (typically oil, water and gas) through porous media. Most of the computational time is spent on solving the resulting linearised systems with a preconditioned Krylov subspace method. The main preconditioning techniques still use the approach introduced by Wallis in 1983, the Constrained Pressure Residual (CPR) preconditioner. In this method, an accurate preconditioner (e.g. AMG) is used for the pressure subsystem, in combination with a cheaper preconditioner (e.g. ILU(0)) for the full system. In this talk, we discuss the details of these two-stage preconditioners and how to treat the coupling between the pressure and the other variables. We also mention the complications when extending these methods to thermal flow. Indeed, the addition of an energy conservation equation introduces cases where the pressure preconditioner fails to fully capture the behaviour of the flow. We consider possible extensions of multi-stage preconditioners for the thermal case.

Adaptive Multipreconditioning for Domain Decomposition

Christophe Bovet *(ONERA)* & Pierre Gosselet *(CNRS, ENS Cachan)* & Augustin Parret-Fréaud *(Safran Tech)* & **Nicole Spillane***(CNRS, École Polytechnique)*

Multipreconditioning is a technique that allows us to simultaneously use several preconditioners within a Krylov subspace solver. It was first introduced in [1] for the conjugate gradient method. The idea is that at each iteration, instead of minimizing the error over one search direction (the preconditioned residual), the error is minimized over an N-dimensional space (spanned by the N preconditioned residuals, where N is the number of preconditioners). Quite naturally, this significantly enlarged search space leads to robust solvers that can converge in a small number of iterations.

Domain decomposition methods are natural candidates for multipreconditioning. Indeed they all share the idea to split the domain into subdomains and then use a sum of local solves (one inside each of the subdomains) as a preconditioner. With multipreconditioning, no sum is performed and instead **each local contribution to the preconditioner is kept separate and used to enlarge the search space**. As an illustration, within multipreconditioned Additive Schwarz the search space at a given iteration (with residual r)

is spanned by $\{R_i^\top A_i^{-1} R_i\, r\}_{i=1,\dots,N}$ (N-dimensional) instead of $\left(\sum_{i=1}^N R_i^\top A_i^{-1} R_i\right) r$ (unidimensional).

The drawback is of course that each iteration becomes more expensive. For this reason an adaptive multipreconditioned conjugate gradient algorithm was introduced in [3] where only some iterations of the Krylov subspace methods are multipreconditioned. In this talk I will discuss how to choose the adaptivity process and show some numerical results [2] on test cases that arise in aircraft engineering.

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Block Preconditioners for an Incompressible Magnetohydrodynamics Problem

Michael Wathen & Chen Greif & Dominik Schötzau *(UBC)*

We consider preconditioning techniques for a mixed finite element discretization of an incompressible magnetohydrodynamics (MHD) problem. Upon discretization and linearization, a 4-by-4 nonsymmetric block-structured linear system needs to be (repeatedly) solved. One of the principal challenges is the presence of a skew-symmetric term that couples the fluid velocity with the magnetic field. Our proposed preconditioner exploits the block structure of the underlying linear system, utilizing and combining effective solvers for the mixed Maxwell and Navier-Stokes subproblems. The preconditioner is based on dual and primal Schur complement approximations to yield a scalable solution method. Large scale numerical results demonstrate the effectiveness of our approach.

Minisymposium M7

Numerical Approximation and Optimization of Agent-based Models

Organisers
Adriano Festa and Dante Kalise

A Semi-Lagrangian scheme for non linear Fokker-Planck equations and applications

Elisabetta Carlini & Francisco J. Silva *(Sapienza Università di Roma)*

We propose a Semi-Lagrangian scheme for non linear Fokker-Planck equations. The scheme is first order, explicit, preserves non-negativity, conserves the mass and allows large time steps. The scheme is written in general dimension, as typical for Semi-Lagrangian scheme, it is free-mesh and it can be applied to solve linear and non linear-non-local problems. We prove a convergence result to the weak solution of the equation.

We apply the scheme to solve a new Hughes-type model, for which we prove an existence result by applying the convergence analysis. The scheme can also be applied to solve Mean Field Games problems, when the coupling is non local. The convergence results apply in dimension 1 for weak solution and in general dimension for smooth solutions. We show numerical simulations of a Lotka-Volterra model, of our new Hughes-type model and of a Mean Field Game model.

Inhomogeneous Boltzmann-Type Equations Modelling Opinion Leadership and Political Segregation

Bertram Düring *(University of Sussex)*

In recent years different kinetic models for socio-economic dynamics like wealth distribution and opinion formation have been proposed. They allow to describe the emergent behaviour of a large number of interacting agents using mathematical tools like Boltzmann-type equations. Most approaches in the literature assume a homogeneous group of agents. To model additional real-world effects, e.g. the influence opinion leaders, one needs to consider inhomogeneous models.

In this talk we discuss inhomogeneous kinetic models for opinion formation, where the opinion formation

process depends on an additional independent variable, e.g. a leadership or a spatial variable. More specifically, we consider: (i) opinion dynamics under the effect of opinion leadership, where each individual is characterised not only by its opinion, but also by another independent variable which quantifies leadership qualities; (ii) opinion dynamics modelling political segregation in 'The Big Sort', a phenomenon that US citizens increasingly prefer to live in neighbourhoods with politically like-minded individuals. Based on microscopic opinion consensus dynamics such models lead to inhomogeneous Boltzmann-type equations for the opinion distribution. We derive macroscopic Fokker-Planck-type equations in a quasi-invariant opinion limit, discuss their numerical discretisation and present results of numerical experiments.

A semi-Lagrangian scheme for Hamilton-Jacobi equations on networks and application to traffic flow models

Adriano Festa *(INSA Rouen)*, Elisabetta Carlini *(Sapienza Rome)* and Nicolas Forcadel *(INSA Rouen)*

In this talk we present a semi-Lagrangian numerical scheme for the approximation of the solution of a Hamilton Jacobi equation on networks. We examine the basic properties of the numerical scheme and we prove convergence and error estimates. We focus on the application of the tools proposed for problems of traffic flows. The good features of the approximation method proposed are validated through some tests both aiming to confirm the theoretical results obtained before to show its effectiveness in solving some applied problems.

A pedestrian flow model with stochastic velocities: microscopic and macroscopic approaches

S. Knapp & S. Göttlich & P. Schillen *(University of Mannheim)*

A well known phenomenon in crowds is the sudden presence of non-moving persons which look at their cell phones, reorientate themselves or watch at a point of interest. This leads to changes in the velocities of the surrounding neighbours, evasive manoeuvre and hence to bottlenecks depending on the crowd density. To include this behaviour into a mathematical model, we consider the well-known social force model by D. Helbing and P. Molnár [1]. Thus, in the literature well studied microscopic model describes the movement of each pedestrian according to his/her destination as well as interaction and obstacle forces.

We embed the mentioned stochastic behaviour into the microscopic pedestrian model by redefining a time-discrete stochastic process which simultaneously implies a microscopic simulation algorithm. Due to the high computational costs of approximating the crowd density for a large number of people, we derive a scalar-type model which approximates the evolution of the crowd density. Finally, the microscopic and the scalar-type model are compared by numerical results in several examples.

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Direct Methods for Bidirectional Formation Control of Vehicle Platoons

Andres Peters *(AC3E, Universidad Técnica Federico Santa María)*

In this talk we present preliminary results on a type of bidirectional formation control architecture. In such architectures almost every member of a platoon is controlled using measurements that contain (directly or indirectly) information from members that are behind them and also from members that are in front of them. Although this architecture has been reported to possess some disadvantages (see for example Seiler et al. (2004); Barooah et al. (2009)), it can be used to allow every member of the platoon to compensate for a disturbance at any particular vehicle.

In particular, the architecture to be studied is a nearest neighbour bidirectional one, where the vehicles use measurements from the immediate predecessor and follower in order to maintain the formation pattern. We present the resulting dynamics of the platoon in the frequency domain as a collection of transfer functions from disturbances to positions. One of the main properties of this interconnection is that the location of the poles of the associated transfer functions will vary with the number of vehicles N, in contrast to what occurs in unidirectional strategies. We will discuss some conditions for establishing the stability of the whole interconnection and some other dynamical properties.

The novelty of the approach presented here lies in the direct method for the computation of the transfer functions from disturbances to vehicle positions. We obtain closed form expressions for these transfer

functions and a way to directly compute the location of their poles. Other works (Barooah et al., 2009) discuss a method to study the behaviour of the least stable pole of a simple bidirectional interconnection. For this they obtain a PDE associated to the limit of a bidirectional platoon of large size. Our method avoids using such approximations and allows for further insight into the possible resulting dynamics.

On numerical simulations of nonlinear continuity equations for interacting particle systems

Helene Ranetbauer & José Carrillo, Marie-Therese Wolfram *(RICAM, Austria)*

In this talk we present a numerical scheme for a class of nonlinear continuity equations, which is based on the gradient flow formulation of an energy functional with respect to the quadratic transportation distance. It can be applied to model interacting particle systems whose dynamics are driven by internal energies, given external potentials and interaction energies. The solver is based on its variational formulation as a gradient flow with respect to the Wasserstein distance. We illustrate this properties with various numerical examples.

Decentralised control of interconnected systems: An interpolation-based approach

Sheila Scialanga & Konstantinos Ampountolas *(University of Glasgow)*

The problem of constrained optimal control of large-scale systems is generally difficult to solve. A first approach is to control the entire network in a centralised fashion. However, such a centralised scheme cannot easily integrate local constraints into the optimal control problem. It can also be computationally expensive due to high dimensions. An alternative avenue is to view the large-scale dynamical system as a decentralised system consisting of a number of interconnected subsystems or neighbourhood systems forming an entity, where each subsystem has independent local constraints, inputs and outputs. The decentralised constrained control problem is to design a controller for each subsystem, where each individual controller uses its local (observed) state vector to generate the local control for the interconnected system.

Decentralised control has been the subject of research in different communities especially in the seventies, and in recent years due to the rapid development of sensing and communication technologies. Nowadays the interest for decentralised control in cities is increased due to the recent advances in vehicle automation and communication technologies that allows for the deployment of cooperative systems with decoupled constraints in connected environments. The primary limitation of decentralised control is that the individual controllers do not (a-priori) coordinate their actions and behaviour, except if appropriate stability criteria are fulfilled. Consequently, local controllers may select individual actions that are locally optimal but that together result in global instabilities. Thus a coordination and connectivity mechanism is necessary to guarantee stability of the overall system. Concluding, the control of interconnected systems with constraints introduces a number of theoretical and computational challenges; on the other hand, considerable system improvements can be achieved in terms of constraint satisfaction, equity and fairness.

In this work, we present a new framework for the decentralised control problem of large-scale interconnected traffic systems with local constraints. We extend an Interpolating-based Control (IC) approach for the constrained decentralised control problem of large-scale interconnected systems. IC is a novel approach that incorporates the state and control constraints in the optimal control problem formulation and significantly reduces the computational effort compared to optimisation-based schemes such as Model Predictive Control (MPC). The main idea behind IC is to blend a global low-gain feedback controller that satisfies the control and state constraints with a user-chosen local high-gain controller that has its positively invariant set satisfying the constraints. For the interpolation a low dimensional Linear Programming problem is solved on-line at each time step. To investigate the performance of distributed IC, we compare the proposed decentralised control with centralised control for simple systems as well as large-scale interconnected traffic systems.

Consensus-Based Global Optimisation

Claudia Totzeck *(TU Kaiserslautern)*

A first-order stochastic algorithm for global optimisation of high-dimensional objective functions will be discussed. The algorithm is inspired by consensus formation and swarm intelligence models. A special feature of the model is that it allows for the passage to the mean-field limit resulting in a nonstandard, nonlocal, degenerate, parabolic PDE. Expoiting tools for PDE analysis, we provide convergence results and a convergence rate on the mean-field level, which transfer to the particle level. In fact, under certain assumptions the algorithm converges arbitrarily close to the global

minimiser of the objective function. Moreover we discuss an extension of the algorithm which approximates Nash-equilibria for cost functions modelling noncooperative games. Numerical results will underline the feasibility of the approaches.

Opinion dynamics over kinetic networks

Mattia Zanella *(Politecnico di Torino)* & Lorenzo Pareschi & Giacomo Albi

In recent years the importance of large scale social networks has grown enormously due to the rapid proliferation of novel communication platforms. The need to handle with millions, and often billions, of vertices implies a considerable shift of interest to large-scale statistical properties of networks which may be described through the methods of the kinetic theory.

In this talk we propose a kinetic description of the agents' distribution over the evolving network which combines an opinion update based on binary interactions between agents with a dynamic creation and removal process of new connections [1]. The number of connections of each agent influences the spreading of opinions in the network, further the way connections are created is influenced by the agents' opinion.

We will study the evolution of the network of connections by showing that its asymptotic behaviour is consistent both with Poisson distributions and truncated power-laws, [2]. In order to study the large time behaviour of the opinion dynamics we derive a mean-field description which allows us to compute exact stationary solutions in some simplified situations. Structure preserving numerical methods are hence employed to describe correctly the large time behaviour of the system, see [3].

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Minisymposium M8

Models and Algorithms for Human Data
Organisers
Des Higham and Ivan Tyukin

Self-Exciting Point Processes for Crime

Craig Gilmour & Des Higham *(University of Strathclyde)*

The question of how crime spreads is an important issue for police and society alike, with some crime types displaying highly clustered sequences in time and space. It has been proposed that certain types of crime, such as burglary, gang crime and gun violence [1,2], take place in highly clustered event sequences, and therefore can be modelled in much the same way that seismic events are, where earthquakes increase the risk of aftershocks occurring in close proximity to the original earthquake.

Self-exciting point processes can be used in situations where the occurrence of an event increases the chances of a subsequent event happening, and can be defined by their *conditional intensity function*

$$\lambda(t) = \lim_{\Delta t \to 0} \frac{\mathbb{E}(N(t, t+\Delta t)|\mathcal{H}_t)}{\Delta t},$$

where $\mathcal{H}_t$ is the history of the process prior to t, and $N(t, t+\Delta t)$ describes the number of points observed in an interval after t.

The Hawkes process is a self-exciting point process whose conditional intensity increases in the aftermath of an event [3]. The conditional intensity function can be given as

$$\lambda(t) = \mu + \sum_{t_i < t} g(t - t_i),$$

where we consider μ to be the background rate, and g to be a triggering function which increases the intensity of the process in the aftermath of an event. Traditionally a parametric form of g has been used, e.g. $g(t) = \alpha\omega e^{-\omega t}$ (known as the epidemic type aftershock, or ETAS, model).

In recent years a method called Model Independent Stochastic Declustering (MISD) has been developed, which can find a non-parametric form for the triggering function without any prior assumptions [4]. In this presentation we will propose and analyse a new triggering function, and compare its performance against non-parametric models. We look at issues of calibration, inference and prediction, and give results on real

crime data made publicly available by the Chicago Police Department.

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Self-esteem and Social Networks of Neural Networks

A.N. Gorban *(University of Leicester)*

We study multi-agent neural networks. An agent submits a solution for each task together with the self-esteem. The self-esteem measures how sure it is about this answer. The problem space is separated between the agents during training. A trained agent solves the problems in his areas correctly and with high self-esteem. The problems which are owned by another agents are either solved correctly or incorrectly but with low self-esteem. Such network can develop and learn further by knowledge transfer between agents in a semi-supervised manner. Distribution of the problems between agents could be also presented in a form of a special adaptive coding neural network. The social networks of neural agents are universal tools for problem solving. Some preliminary ideas about separation of the problems between neural agents were published in 1991 [1,2].

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The blessing of dimensionality and the curse of being a mathematician

Jeremy Levesley *(University of Leicester)*

In this talk we will discuss the discrimination problem in high dimensions. We will discuss the problem with using smoothness as a criterion for describing information and how the mathematician desire to know things too well is an obstacle in thinking about the problem - the so called curse of dimensionality. With reference to the concentration of measure phenomenon we will talk about how the task of building a new classifier from an old one, where a new piece of information is introduced is straightforward. This will contrast with the view that a new piece of information requires complete relearning of the system.

Generalized cognitive maps for decision-making in dynamic situations

V.A. Makarov, J.A. Villacorta-Atienza, C. Calvo & A. Sanchez *(Universidad Complutense de Madrid) S. Lobov (Lobachevsky State University of Nizhny Novgorod)*

The fundamental bases of how our brain represents dynamic situations and makes decisions remain largely unknown. Here we consider two different problems: agent navigation and limb movement in dynamic situations. We solve both problems on an abstract cognitive level by constructing generalized cognitive maps (GCM) that enable an efficient decision-making in complex situations. A GCM provides a trajectory that can be followed by an agent or a limb, which ensures a collision-free movement and reaching a target. The approach feasibility is illustrated in numerical simulations and experimentally with robots in real-life scenarios. Finally we discuss how the static nature of GCMs enables learning and automation of sophisticated cognitive behaviors exhibited by humans. We present new behavioral data collected on humans that provide support for the GCM concept.

This work was supported by the Spanish Ministry of Economy and Competitiveness under grant FIS2014-57090-P (theoretical development) and by the Russian Science Foundation under project 151210018 (experi-

mental verification in robot).

One-shot learning and knowledge transfer in Artificial Intelligence Systems

Ivan Tyukin & Alexander Gorban *(University of Leicester)*

We consider the fundamental question: how a legacy student Artificial Intelligent (AI) system could learn from a legacy teacher AI system or a human expert without complete re-training and, most importantly, without requiring significant computational resources. Here learning is understood as an ability of one system to mimic responses of the other and vice-versa. We call such learning as Artificial Intelligence knowledge transfer. We show that if a) internal variables of the student Artificial Intelligent system have the structure of an n-dimensional topological vector space, b) pre-existing knowledge is more or less evenly represented in a bounded domain of this space, and c) n is sufficiently high then, with probability close to one, the required knowledge transfer can be implemented by simple cascades of linear functionals. In particular, for n sufficiently large, with probability close to one, the student system can successfully and non-iteratively learn $k \ll n$ new examples from the teacher (or correct the same number of mistakes) at the cost of just few additional inner products. The concept is illustrated with examples of 1) knowledge transfer from a human expert to a pre-trained convolutional neural network and 2) from a pre-trained convolutional neural network to a simple linear Histograms of Oriented Gradients (HOGs) - SVM classifier.

Minisymposium M9

Numerical Methods for Interface and Multiphysics Problems

Organisers

Gabriel Barrenechea and Heiko Gimperlein

On the Stokes equation in a periodically perforated domain with slip boundary condition of friction type on the interface

Leonardo Baffico *(Laboratoire de Mathématiques N. Oresme UMR 6139, Université de Caen Normandie - CNRS)*

We study the Stokes equation posed in a periodically perforated domain with small period $\varepsilon > 0$. On the interface between the fluid and the holes, instead of the classical no-slip condition, we use a slip boundary condition of friction type. This problem could model the flow of an incompressible Newtonian viscous fluid in a porous media when slip on the fluid-solid interface could happen, if some conditions are reached. Based on *a priori* estimates for the velocity and pressure, we use two-scale asymptotic expansions to formally deduce a two-scale homogenized problem. Then, using the incompressibility of the fluid, we derive a non-linear Darcy equation for the macroscopic pressure. Finally, we present a numerical strategy to solve this non-linear problem based on a quasi-Newton method and on the resolution of periodic Stokes problems, with slip boundary condition, in the reference cell. Some open questions about the two-scale convergence, when $\varepsilon \to 0$, will be addressed at the end of the talk.

Fluid-structure interaction simulations of magnetic drug targeting

Giacomo Capodaglio & Eugenio Aulisa & Sara Calandrini *(Texas Tech University)*

I will present fluid-structure interaction (FSI) simulations of magnetic drug targeting (MDT) in blood flows. In such procedureS, magnetic particles are attached to a drug injected in the body. This allows an external magnet to direct the particles to a specific target. The goal is to minimize the healthy tissue affected by the treatment and to maximize the number of particles that reach the target. This is quantified by the capture efficiency, the ratio between the number of particles that don't leave the domain and the number of particles injected. For the numerical simulations, we used the in-house finite element library FEMuS (https://github.com/FeMTTU/femus) where the FSI solver and the particle tracking algorithm are implemented. Such an algorithm has been developed by the authors and is designed to work with fully unstructured finite element grids and parallel applications. I will first compare our numerical results to existing results obtained under the assumption of undeformable walls to investigate the influence of the solid deformations on the capture efficiency. I will conclude with a realistic biological application, where MDT-FSI simulations are performed on a carotid artery where the magnetic field is produced by a superconducting magnet.

Boundary elements for contact problems: stabilisation and time domain

Heiko Gimperlein *(Heriot-Watt University and University of Paderborn)*

Contact and friction naturally arise in mechanics at the interface of two materials. We discuss the numerical analysis of the corresponding variational inequalities, or PDE with inequality conditions at the interface, both for time-independent and dynamic problems.

In the time-independent case adaptive boundary element procedures provide an efficient and extensively investigated tool for their numerical solution. We discuss efficient mixed *hp* methods based on a least squares stabilisation and provide both an a priori and a posteriori error analysis for non-penetration and friction contact. The a posteriori error estimates give rise to *hp* adaptive mesh refinement procedures.

For contact in the time domain, even the existence of solutions is not known except for the case of the wave equation with a flat contact area. We present a first a priori and a posteriori error analysis for the boundary element discretisation of such dynamic contact problems in the case where the existence of solutions is known. An outlook considers the stabilisation of the space-time methods.

Numerical results illustrate the efficiency of our methods for both time-independent and dynamic contact.

A stabilised finite element method for a fictitious domain problem allowing small inclusions

Cheherazada González Aguayo & Gabriel R. Barrenechea *(University of Strathclyde)*

The purpose of this work is to approximate numerically elliptic and parabolic partial differential equations posed on domains with small perforations (or inclusions). The approach is based on the fictitious domain method, and since the method's interest lie in the case in which the geometrical features are not resolved by the mesh, we propose a stabilised finite element method. The stabilisation term is a simple, non-consistent penalisation, that can be linked to the Barbosa-Hughes approach. Stability and optimal convergence are proved in the elliptic case. Futhermore, we present the full analysis for transient problems on complicated domains through fictitious domain methods. We prove unconditional stability of the solution and Lagrange multipliers, and optimal convergence for the transient heat equation when the initial datum is chosen as a certain Ritz-type projection. Numerical results confirm the theory.

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A-posteriori error estimator for a strongly conservative finite element method for Stokes-Darcy coupling equation

Arbaz Khan & Guido Kanschat *(Interdisziplinäres Zentrum für Wissenschaftliches Rechnen (IWR), Ruprecht-Karls-Universität)*

Computing the numerical solution of the coupling of fluid flow with porous media flow, in which the respective interface conditions are given by balance of normal forces, mass conservation and Beavers-Joseph-Saffman law, is a very active research area. These problems have many important applications such as the modelling of groundwater contamination through streams and filtration problems.

It is the aim of this talk to present the a-posteriori

error estimator for a strongly conservative finite element method for the coupling of fluid flow with porous media flow in $2-D$. These flows are governed by the Stokes and Darcy equation with the Beavers-Joseph-Saffman interface condition. We use the divergence-conforming velocity space with matching pressure space (such as Raviart-Thomas spaces) in discrete level. A reliable and efficient residual-based a-posteriori error estimator is derived for the couple problem. Specific numerical experiments are given to validate the theoretical properties of this estimator and show the capability of the corresponding adaptive algorithm to localize the singularities of the solution.

Minisymposium M10

Numerical Methods for PDE-Constrained Optimization

Organisers

Dante Kalise and Tyrone Rees

A posteriori error estimation for finite element approximations of a PDE–constrained optimization problem in fluid dynamics

Alejandro Allendes & Enrique Otárola & Richard Rankin *(Universidad Técnica Federico Santa María)*, and Abner J. Salgado *(University of Tennessee)*

We present a unifying framework to obtain a posteriori error estimators for PDE–constrained optimization problems involving linear models in fluid dynamics as a state equation; control constraints are also considered. We propose a scheme that is based on the discretization of the associated optimality system and discretize the state and adjoint equations with either standard or stabilized finite element methods. When stabilized methods are considered, no a priori relation between the stabilization terms for the state and adjoint equations is required. The proposed error estimators are thus defined as the sum of three contributions: a contribution that accounts for the discretization of the optimal control variable and two contributions associated with the discretization of the state and adjoint equations. Under certain assumptions on the latter two contributions we derive the reliability and efficiency of the proposed error estimators. We review a residual–type error estimator and a fully computable one that provides a bound for the error that is free of unknown constants.

References

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Low-rank solution of the optimal control problem for random Navier-Stokes equations

Sergey Dolgov *(University of Bath)* & Peter Benner, Akwum Onwunta and Martin Stoll (Max Planck Institute)

Controlling of incompressible fluid flows is a timely but computationally demanding problem. It is even more challenging when some data (such as the inflow) are not known exactly, but can only be introduced as random fields. We consider this stochastic optimal control problem, with a deterministic least squares objective functional with a classical Tikhonov regularization, but the constraints given by the Navier-Stokes equations with a stochastic inflow. The stochasticity is parametrized by auxiliary variables and discretized by the stochastic Galerkin finite element method. This turns the optimality conditions into a prohibitively high dimensional system of equations with a saddle point structure. To reduce the number of degrees of freedom, we approximate all functions by low-rank decompositions with separated variables. The optimality equations are solved via an alternating iteration with respect to different factors of the low-rank representation directly, such that the full model is never constructed. We show that the solution of the vorticity minimization problem with a distributed control admits an approximation with ranks that depend modestly on model and discretization parameters even for high Reynolds numbers. As a result, the low-rank solution leads to orders of magnitude savings in terms of memory and computational costs.

Proximal methods for stationary Mean Field Games with local couplings

Dante Kalise *(Johann Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria)* & Luis Bricenõ-Arias & Francisco J. Silva

In this talk we address the numerical approximation of Mean Field Games with local couplings. For power-like Hamiltonians, we consider both unconstrained and constrained stationary systems with den-

sity constraints in order to model hard congestion effects. For finite difference discretizations of the Mean Field Game system, we follow a variational approach. We prove that the aforementioned schemes can be obtained as the optimality system of suitably defined optimization problems. Then, the variational problem is cast as a convex optimization problem for which we study and compare several proximal type methods. These algorithms have several interesting features, such as global convergence and stability with respect to the viscosity parameter, which can eventually be zero. We assess the performance of the methods via numerical experiments.

Preconditioned Iterative Methods for Optimal Transport Problems

John Pearson *(University of Kent)*

The problem of optimal transport is a longstanding and active area of research in applied mathematics and engineering, and a key application of the field of PDE-constrained optimization. In this talk, we consider a particular transport equation arising from the modelling of image metamorphosis. When solving such problems accurately on the discrete level, it is important to develop fast and efficient numerical algorithms which may be readily applied to solve the resulting matrix systems.

We present new preconditioned iterative methods which may be used to tackle the large and sparse saddle point systems arising from these problems. Crucial to the effectiveness of our methods are potent approximations of the $(1,1)$-block and Schur complement of the matrices obtained. We demonstrate the applicability of our techniques to finite difference discretizations of the nonlinear system of PDEs, as well as to a new radial basis function strategy which we also present. We consider both the theoretical rate of convergence of our solvers, and the results obtained from the solution of practical numerical examples.

On the feedback stabilization to trajectories for semilinear parabolic equations

Sérgio S. Rodrigues & Duy Phan *(RICAM-OeAW)*

Recent results on the feedback stabilization to trajectories for parabolic equations by means of a finite number of actuators are presented. After linearization around the targeted time-dependent trajectory one has to deal with the stabilization of a nonautonomous linear parabolic equation. Dealing with the nonautonomous case requires tools different from the spectral properties used to deal with the autonomous one. Both internal and boundary actuators will be considered. A finite element based discretization of such problems is proposed/discussed, and results of the respective numerical simulations are presented.

Approximation of normal vector fields with applications to shape optimisation

Kevin Sturm & Alberto Paganini *(Johann Radon Institute for Computational and Applied Mathematics (RICAM))*

In this talk I discuss the approximation of normal vector fields defined on the boundary of a domain in dimension two. For this purpose we introduce so-called weakly normal basis functions in reproducing kernels Hilbert spaces. These normal functions enjoy several nice properties and are tailored to shape optimisation problems.

Minisymposium M11

Learning functions from data
Organisers
Andrew Stuart and Aretha Teckentrup

Kernel methods for parametric pdes

Christian Rieger *(Bonn University)*

In many applications, one uses stochastic modeling to incorporate unresolved physical properties into existing models, which are often formulated as partial differential equations. Numerical discretizations of the stochastic influences often lead to parametric partial differential equations. Without any further assumptions, the parameters stem from a high or infinite dimensional space, and hence every numerical method would suffer from the so called curse of dimension. Due to regularity theory of the underlying pde, one can in many situations identify additional structures (e.g. regularity, decay of importance of dimensions) which allow reasonable computations despite the nominally high dimension of the parameter space. We show how such structures can be incorporated into reproducing kernels or covariance functions. Given such kernels we discuss regularized reconstruction methods and their deterministic a priori error analysis.

This is partly based on joint work with Michael Griebel

(Bonn).

Gaussian process emulators in Bayesian inverse problems

Aretha Teckentrup & Andrew Stuart *(University of Edinburgh & Alan Turing Institute)*

A major challenge in the application of sampling methods in Bayesian inverse problems is the typically large computational cost associated with solving the forward problem. To overcome this issue, we consider using a Gaussian process emulator to approximate the forward map. This results in an approximation to the solution of the Bayesian inverse problem, and more precisely in an approximate posterior distribution.

In this talk, we analyse the error in the approximate posterior distribution, and show that the approximate posterior distribution tends to the true posterior as the accuracy of the Gaussian process emulator increases.

Learning Sparse Additive Models with Interactions in High Dimensions

Hemant Tyagi, Anastasios Kyrillidis, Bernd Gärtner & Andreas Krause *(Alan Turing Institute and University of Edinburgh)*

A function $f : \mathbb{R}^d \to \mathbb{R}$ is a Sparse Additive Model (SPAM), if it is of the form $f(\mathbf{x}) = \sum_{l\in\mathcal{S}} \phi_l(x_l)$ where $\mathcal{S} \subset [d]$, $|\mathcal{S}| \ll d$. Assuming ϕ's, $\mathcal{S}$ to be unknown, there exists extensive work for estimating f from its samples. In this work, we consider a generalized version of SPAMs, that also allows for the presence of a sparse number of *second order interaction terms*. For some $\mathcal{S}_1 \subset [d], \mathcal{S}_2 \subset \binom{[d]}{2}$, with $|\mathcal{S}_1| \ll d, |\mathcal{S}_2| \ll d^2$, the function f is now assumed to be of the form: $\sum_{p\in\mathcal{S}_1} \phi_p(x_p) + \sum_{(l,l')\in\mathcal{S}_2} \phi_{(l,l')}(x_l, x_{l'})$. Assuming we have the freedom to query f anywhere in its domain, we derive efficient algorithms that provably recover $\mathcal{S}_1, \mathcal{S}_2$ with *finite sample bounds*. Our analysis covers the noiseless setting where exact samples of f are obtained, and also extends to the noisy setting where the queries are corrupted with noise. For the noisy setting in particular, we consider two noise models namely: i.i.d Gaussian noise and arbitrary but bounded noise. Our main methods for identification of $\mathcal{S}_2$ essentially rely on estimation of sparse Hessian matrices, for which we provide two novel compressed sensing based schemes.

Multiscale Radial Basis Functions

Holger Wendland *(University of Bayreuth)*

Radial basis functions (RBFs) are a popular meshfree discretisation method. They are used in various areas comprising, for example, scattered data approximation, computer graphics, machine learning, aeroelasticity and the geosciences.

The approximation space is usually formed using the shifts of a fixed basis function. This simple approach makes it easy to construct approximation spaces of arbitrary smoothness and in arbitrary dimensions.

Multiscale RBFs employ radial basis functions with compact support. In contrast to classical RBFs they do not only use the shifts of a fixed basis function but also vary the support radius in an orderly fashion. If done correctly, this leads to an extremely versatile and efficient approximation method.

In this talk, I will discuss the basic ideas of multiscale RBFs, I will give and analyse an explicit algorithm for the reconstruction of multivariate functions from scattered data. After that, I will discuss how multiscale RBFs can be used for data compression, for the resolution of different scales in the target function and, if time permits, how they can be used to solve partial differential equations numerically.

This talk is based upon joint work with Thong Le Gia, Ian Sloan (University of New South Wales, Sydney, Australia) and Patricio Farrell (WIAS, Berlin, Germany).

Learning functions from data under supremum loss: Wavelets, basis splines and uncertainty quantification

William Weimin Yoo & Aad van der Vaart *(Leiden University)*

In statistics and numerical analysis, functions are estimated or learned by optimizing loss functions, with the most commonly used being the integrated mean square error and other distance measures based on the L_2-norm. These measures however only guarantee performance "on the average", and in some applications, a stronger control on the error is needed with performance guaranteed uniformly across the function's domain. This then calls for the supremum norm to be used in quantifying loss. In this talk, I will discuss using the supremum loss to learn regression func-

tion from a Bayesian point of view. In particular, I will talk about adaptive procedures based on wavelet and basis spline projections. Other topics of interest that I will touch upon include numerical computation using discrete wavelet transforms, and uncertainty quantification in the function learning process.

Minisymposium M12

Recent Developments in Uncertainty Quantification
Organiser
Ivan Graham

On the design and performance of adaptive stochastic Galerkin methods

Alex Bespalov *(University of Birmingham)*

This talk highlights recent developments in designing efficient adaptive algorithms for computing stochastic Galerkin finite element approximations of solutions to elliptic PDE problems with random inputs. We consider a class of elliptic PDEs where the underlying differential operator has affine dependence on a large, possibly infinite, number of random parameters. We will discuss different strategies for designing an algorithm that combines adaptive local mesh refinement on the spatial domain with adaptive selection of polynomial approximations on the parameter domain. We build upon the algorithm developed in [A. Bespalov and D. Silvester, SIAM J. Sci. Comput., 38(4): A2118–2140, 2016], that relies on effective estimates of the error reduction for enhanced approximations, but now employ Dörfler marking for both spatial and parametric approximations. We compare numerically the performance of different adaptive strategies in terms of convergence, computational times, generated local mesh refinements on the spatial domain, and evolution of polynomial approximations on the parameter domain.

Lower set supported sparse estimation and application to uncertainty quantification for PDEs using compressed sensing

Stéphane P.A. Bordas, **Stéphane Chrétien** & Franz Chouly
(University of Luxembourg, **NPL***, Université Bourgogne Franche-Comté)*

Uncertainty quantification is a field of fast growing interest in the numerical analysis of certain (systems of) partial differential equations (PDEs)

$$\mathcal{L}(u; x, z) = 0$$

where u is the unknown, $x \in \mathbb{R}^p$ is the physical variable (e.g. spatial coordinates) and $z \in \mathbb{R}^d$ is a vector of parameters. In practice, one is often interested in modelling the impact of varying parameters z on the value of $f(u)$, where $f(\cdot)$ is a given functional of the solution u, associated to a quantity of interest, relevant for practitioners (f can genuinely be the identity). In other words, we are interested in approximating the mapping $z \mapsto f(u)(x, z)$. In the setting recently developed by several authors including Adcock, Andreev, Nobile, Maday, Chkifa, Cohen, Schwab, etc, we are simply given some values $f(z^{(1)}), \ldots, f(z^{(n)})$ at randomly sampled points $z^{(1)}, \ldots, z^{(n)}$ and one usually approximates f using a basis of multivariate orthonormal polynomials

$$f(z) = \sum_{i \in I} c_i \phi_i(z).$$

Most often, the measure used for sampling is the same as the measure with respect to which the polynomials are orthogonal. For an overview of tensor based modelling techniques, we refer the reader to Grasedyck, L., Kressner, D. & Tobler, C. (2013). (A literature survey of low rank tensor approximation techniques. GAMMMitteilungen, 36(1), 53-78), and Chinesta, F., Ladevèze, P. & Cueto, E. (2011) (A short review on model order reduction based on proper generalized decomposition. Archives of Computational Methods in Engineering, 18(4), 395)

One of the main results obtained by Chkifa, Cohen and Schwab (*High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs, FoCM 2014*) is that for a wide class of parametrised PDEs, the vector c is sparse and the sparsity pattern bears a special hierarchical structure. The set of supports of such c's is denoted the family of *lower sets*. These sets are characterised by the fact that if a multi-index i belongs to such a set S, then any componentwise smaller multi-index also belongs to S.

Using the paradigm of Compressed Sensing, the estimation of c can be performed using a penalised least-squares approach where the penalty enforces the support of the estimator $\hat{c}$ to be a lower set. The structure of lower sets can be leveraged in order to apply the method of Obozinski and Bach, (*A unified perspective on convex structured sparsity: Hierarchical, symmetric, submodular norms and beyond, preprint 2016*) for providing an associated convex penalisation.

One of the main drawbacks of the convexifications of the combinatorial penalties proposed recently is their

computational complexity when dealing with the practical implementation. Our main contribution is to provide an efficient algorithm for estimating c from $z^{(1)}, \ldots, z^{(n)}$ based on an extension of Matching Pursuit (Mallat, S. G. and Zhang, Z. *Matching Pursuits with Time-Frequency Dictionaries. IEEE Transactions on Signal Processing. 1993, pp. 3397–3415*). A theoretical analysis will be provided, as well as numerical results on a simplified model problem inspired by real problems in (bio)mechanics.

Applying quasi-Monte Carlo integration to a parametrised elliptic eigenproblem

Alec Gilbert & Ivan Graham, Frances Kuo, Rob Scheichl, Ian Sloan *(UNSW Sydney)*

In this talk we study an elliptic eigenproblem, with a random coefficient that can be parametrised by infinitely many stochastic parameters. The randomness in the coefficient also results in randomness in the eigenvalues and corresponding eigenfunctions. As such, our quantity of interest is the expected value, with respect to the stochastic parameters, of the smallest eigenvalue, which we formulate as an integral over the infinite-dimensional parameter domain. Our approximation involves three steps: truncating the stochastic dimension, discretising the spatial domain using finite elements and approximating the now finite but still high-dimensional integral.

To approximate the high-dimensional integral we use quasi-Monte Carlo (QMC) methods. These are deterministic or quasi-random quadrature rules that can be proven to be very efficient for the numerical integration of certain classes of high-dimensional functions. QMC methods have previously been applied to linear functionals of the solution of a similar elliptic source problem; however, because of the nonlinearity of eigenvalues the existing analysis of the integration error does not hold in our case. We show that the minimal eigenvalue belongs to the spaces required for QMC theory, outline the approximation algorithm and provide numerical results.

A high dimensional UQ problem for neutron transport and its solution using multilevel sampling

Ivan Graham, Matthew Parkinson & Robert Scheichl *(University of Bath)*

Transport equations describe the transport of radiation in the presence of absorption, scattering and possibly fission processes. They have applications in optics, astrophysics and nuclear safety – in the latter case the equation is known as the neutron (or Boltzmann) transport equation. We describe modern variants of Monte Carlo methods for Uncertainty Quantification (UQ) of the neutron transport equation, when it is approximated by the discrete ordinates method with diamond differencing. We focus on the mono-energetic 1D in space and 1D in angle slab geometry problem, with isotropic scattering, where the cross-sections are log-normal correlated random fields of possibly low regularity. We describe the theory and practice of algorithms for quantifying the uncertainty of a linear functional of the scalar flux, using Monte Carlo and quasi-Monte Carlo methods, and their multilevel variants. Numerical experiments show the effectiveness of the hybrid solver and the gains that are possible through quasi-Monte Carlo sampling and multilevel variance reduction. For the multilevel quasi-Monte Carlo method, we observe gains in the computational ε-cost of up to 2 orders of magnitude over the standard Monte Carlo method, and we explain this theoretically. Experiments on problems with up to several thousand stochastic dimensions are included.

Analysis and application of stochastic collocation methods for Maxwell's equations with random coefficients

Jichun Li & Zhiwei Fang *(University of Nevada Las Vegas)*

In this talk, we will present the development and analysis of the stochastic collocation method for solving the time-dependent Maxwell's equations with random coefficients and subject to random initial conditions. We provide a rigorous regularity analysis of the solution with respect to the random variable. To our best knowledge, this is the first theoretical results derived for the stochastic Maxwell's equations. The rate of convergence is proved depending on the regularity of the solution. Numerical results are presented to confirm the theoretical analysis.

Major references are:
[1] J. Li and Y. Huang, Time-Domain Finite Element Methods for Maxwell's Equations in Metamaterials, *Springer Series in Computational Mathematics*, **vol. 43**, Springer, 2013.
[2] J. Li and Z. Fang, Analysis and application of stochastic collocation methods for Maxwell's equations with random coefficients (under review).

A Reduced Basis Solver for Stochastic Galerkin

Matrix Equations

Catherine Powell & Valeria Simoncini & David Silvester *(University of Manchester)*

Stochastic Galerkin finite element methods (SGFEMs) are a popular alternative to sampling methods for solving PDEs with random inputs. Unlike sampling methods, which require the solution of many deterministic problems, SGFEMs yield huge linear systems of equations with coefficient matrices that have a characteristic Kronecker product structure. By reformulating the systems as multiterm linear matrix equations, we have developed [see: C.E. Powell, D. Silvester, V.Simoncini, An efficient reduced basis solver for stochastic Galerkin matrix equations, SIAM J. Comp. Sci. 39(1), pp A141-A163 (2017)] a memory-efficient solution algorithm which generalizes ideas from rational Krylov subspace approximation. The new approach determines a low-rank approximation to the solution matrix by performing a projection onto a reduced approximation space (that is iteratively augmented with problem-specific basis vectors) and provides an efficient solution strategy whose convergence rate is independent of the spatial approximation. Moreover, it requires far less memory than standard preconditioned Krylov methods (such as mean-based preconditioned CG) applied to the Kronecker formulation of the linear systems. For test problems consisting of elliptic PDEs with random coefficients, we are able to solve $O(10^9)$ equations on a standard desktop computer quickly and efficiently.

Using Surrogate Models to Accelerate Bayesian Inverse Uncertainty Quantification

James Rynn & Catherine Powell & Simon Cotter *(University of Manchester)* & Louise Wright *(National Physical Laboratory)*

In this talk we consider inverse uncertainty quantification for the laser flash experiment. We assume the change in temperature of a material is modelled by the transient heat equation. Inputs such as the diffusion coefficient, boundary condition and source term considered unknown. We take the Bayesian approach, utilising Markov chain Monte Carlo (MCMC) methods to sample from the posterior distribution of the unknowns given observations of the temperature made during experimentation.

MCMC algorithms require many calculations of the posterior density. Each evaluation of the posterior density requires an evaluation of the forward model, which in this setting is the numerical solution of a time–dependent PDE. This requirement results in a computationally intensive routine, often taking days to achieve a desired Monte Carlo error in the quantities of interest. Although computationally intensive, such a routine is preferable to cheaper optimisation approaches which provide no quantification of the uncertainty, only a fitted best value.

We analyse the validity of using a surrogate model within an MCMC routine to reduce the computational cost. Specifically, we evaluate a single stochastic Galerkin finite element solution to the PDE in place of repeatedly computing deterministic finite element solutions within an MCMC routine. Investigations into how both the speed and accuracy of the approximation of the posterior are affected by this replacement are presented.

Stochastic collocation methods for stability analysis of dynamical systems

David Silvester *(University of Manchester)*

Eigenvalue analysis is a well-established tool for stability analysis of dynamical systems. However, there are situations where eigenvalues miss some important features of physical models. For example, in models of incompressible fluid dynamics, there are examples where linear stability analysis predicts stability but transient simulations exhibit significant growth of infinitesimal perturbations. In this study, we show that an approach similar to pseudo-spectral analysis can be performed inexpensively using stochastic collocation methods and the results can be used to provide quantitative information about the nature and probability of instability.

This is joint work with Howard Elman.

High-dimensional integration of kinks and jumps – smoothing by preintegration

Ian H Sloan *(UNSW Sydney, Australia)*

In many applications, including option pricing, integrals of d-variate functions with "kinks" or "jumps" are encountered. (Kinks describe simple discontinuities in the derivative, jumps describe simple discontinuities in function values.) The standard analyses of sparse grid or Quasi-Monte Carlo methods fail completely in the presence of kinks or jumps, yet the observed performance of these methods can remain rea-

sonable.

In joint papers with Michael Griebel and Frances Kuo we sought an explanation by showing that many terms of the ANOVA expansion of a function with kinks can be smooth, because of the smoothing effect of integration. In particular, we showed that 1-dimensional integration of a non-smooth function on R^d with respect to a well chosen variable, say x_j, can result in a smooth function of $d-1$ variables.

In recent joint work with Andreas Griewank, Hernan Leovey and Frances Kuo we have extended the theoretical results from kinks to jumps, and have turned "preintegration" into a practical method for evaluating integrals of non-smooth functions over d-dimensional Euclidean space. In this talk I will explain both the method and the ideas behind "smoothing by preintegration".

Minisymposium M13

Advances in the robust solution of singularly perturbed differential equations

Organisers

Natalia Kopteva, Torsten Linß and Niall Madden

Fully-discrete methods for mixed finite-element approximations of the time-dependent Navier-Stokes equations with grad-div stabilization

Bosco García-Archilla, J. de Frutors, V. John & J. Novo *(Universidad de Sevilla)*

We consider a fully-discrete numerical method for the time-dependent Navier-Stokes equations where inf-sup stable finite elements with grad-div stabilization are used for the spatial discretization, and the backward Euler method is used for time discretization. We analyze the method without assuming (unrealistic) nonlocal compatibility conditions at the initial time, so that the solution cannot be assumed to have more than second order derivatives (in space) which are bounded up to the initial time, or more than first order bounded derivatives (in time). We obtain error bounds with constants that do not depend on the inverse of the viscosity parameter. To our knowledge, this is the first time that such viscosity-independent bounds are obtained for a fully discrete method under realistic assumptions. The decay rate in h (mesh-size) is the same as under more benign assumptions, but loses one half order in the time step. The results we present are a summary of those presented in [1].

References

[1] J. de Frutos, B. García-Archilla, V. John and J. Novo, Analysis of the grad-div stabilization for the time-dependent Navier-Stokes equations with inf-sup stable finite elements, (submitted).

Numerical solution of convection-diffusion problems on annular domains

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

We examine numerical methods for the solution of convection diffusion problems on annular domains. The methods involve polar coordinates, upwinding, piecewise-uniform Shishkin meshes in the radial direction, and possibly some refinement in the axial direction. We examine computationally the effect of relaxing constraints on the data which are required to obtain parameter-uniform error bounds and briefly consider the application of the methods to similar domains with non-circular boundaries.

The numerical method is a variation of that considered in [1, 2], where the domain is circular and [3] in which numerical solutions are also obtained on annular domains.

References

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[3] A. F. Hegarty and E. O' Riordan, Numerical methods for singularly perturbed problems on non-rectangular domains, *Proceedings of BAIL 2016 conference.*

Numerical resolution of time dependent diffusion-reaction systems: a splitting by components

J. C. Jorge & C. Clavero *(Universidad Pública de Navarra)*

In this talk we propose and analyze an efficient and uniformly convergent method for solving linear 1D parabolic singularly perturbed systems of reaction-diffusion type, which are coupled in the reaction term. We will focus our attention on the problems which have several small diffusion parameters with different magnitudes; in these cases, in general, overlapping boundary layers appear at both end points of the spatial domain. The numerical method is constructed by combining the fractional Euler implicit method, together with a splitting-by-components of the diffusion reaction operator, to integrate in time, and the classical central finite difference scheme, defined on a special mesh of Shishkin type, to discretize in space. The use of the fractional Euler method joint to the splitting by components gets that only tridiagonal linear systems must be solved to obtain the numerical solution, reducing considerably the computational cost of the method with respect to other classical implicit methods, which require to solve linear systems with a larger bandwidth. As long as the number of components grows, the proposed splitting method becomes more efficient compared to classical implicit methods. We prove that the proposed method is uniformly convergent of first order in time and almost second order in space. Some numerical experiments are shown in order to illustrate the behavior of our algorithm in practice.

Anisotropic flux equilibration on anisotropic meshes

Natalia Kopteva *(University of Limerick)*

Explicitly and fully computable a posteriori error estimates in the energy norm are given in the energy norm on reasonably general anisotropic meshes (see a recent paper [6] for further details).

We consider linear finite element approximations to singularly perturbed semilinear reaction-diffusion equations of the form $-\varepsilon^2\triangle u+f(x,y;u)=0$, with $0<\varepsilon\leq 1$, posed in polygonal domains.

A posteriori error bounds are obtained employing a certain combination of explicit flux reconstruction and flux equilibration; see, e.g., [1, 2] for the case of shape-regular meshes.

Our approach differs from the previous work in a few ways.

- The fluxes are equilibrated within a local patch using anisotropic weights depending on the local, possibly anisotropic, mesh geometry.
- Prior to the flux equilibration, divergence-free corrections are introduced for pairs of anisotropic triangles sharing a short edge.
- A certain anisotropic quadrature is used on anisotropic elements. This is motivated by some observations made in [3], and also enables us to drop some mesh assumptions made in [4, 5].
- Our estimator is explicitly and fully computable in the sense that it involves no unknown error constants (unlike other estimators on anisotropic meshes, such as in [4, 5]).
- An upper bound for our estimator involves no matching functions (which depend on the unknown error). In fact, the error constant C in our upper bound is independent not only of the diameters and the aspect ratios of mesh elements, but also of the small perturbation parameter ε.

References

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anisotropic meshes, April 2017, submitted for publication, arXiv:1704.04404.

Collocation for singularly perturbed boundary-value problems

Torsten Linß & Goran Radojev & Helena Zarin *(FernUniversität in Hagen)*

A short summary of recent research into maximum-norm error estimates for collocation methods applied to singularly perturbed boundary-value problems of reaction-diffusion type will be given. Both a priori and a posteriori error bounds will be presented.

Parameter robust solvers for singularly perturbed differential equations

Niall Madden, Scott MacLachlan & Thái Anh Nhan *(National University of Ireland, Galway)*

We consider the numerical solution of singularly perturbed ordinary and partial differential equations. These problems feature a small perturbation parameter, usually denoted ε, multiplying the highest derivatives. Their solutions typically feature boundary and/or interior layers. Numerous specialised methods have been proposed for computing solutions to these problems, most often involving specially designed, highly anisotropic layer-adapted meshes. A method is called *parameter robust* if its accuracy is independent of ε for a fixed number of degrees of freedom. Simply put, the computational cost of a robust method achieving a fixed accuracy should be independent of ε. When computing numerical solutions to partial differential equations using, for example, a standard finite element method, most of this cost is incurred when solving associated linear system. Surprisingly, the time required to solve such linear system depends adversely on ε, *even when a direct solver is used*. We will examine this phenomenon, and then propose strategies based on iterative solvers. The meshes are used for singularly perturbed problems are very fine, and can have large aspect ratios so, not surprisingly, the linear systems are ill-conditioned. Careful design of suitable preconditioners is necessary in order to solve them in a way that is robust, with respect to the perturbation parameter, and efficient. We consider several approaches, including a *boundary layer preconditioner*, in the style of that used for a finite-difference method in [1].

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Singularly perturbed convection-diffusion problems posed on an annulus

Eugene O'Riordan & Alan Hegarty *(Dublin City University)*

A finite difference method is constructed for singularly perturbed convection diffusion problems posed on an annulus. The method involves combining polar coordinates, upwinding and a piecewise-uniform Shishkin mesh in the radial direction. Constraints are imposed on the data in the vicinity of certain characteristic points to ensure that interior parabolic layers do not form within the annulus. Under these constraints, a theoretical parameter-uniform error bound can be established.

Balanced-norm error estimates for sparse grid finite element methods

Stephen Russell & Martin Stynes *(Beijing Computational Science Research Center)*

Error estimates for standard finite element methods (FEMs), and their sparse grid variants, applied to singularly perturbed reaction-diffusion problems, $-\varepsilon^2\Delta u + cu = f$, are typically quantified in the usual energy norm:

$$\|u\|_\varepsilon = \left\{\varepsilon^2|u|^2 + \|u\|_0^2\right\}^{1/2}.$$

However, it can be argued that for problems of this type, this energy norm is too weak to capture adequately the behaviour of the boundary layers that appear in the solution. That is, for a typical layer

component ϕ of the solution u to such problems, one has that $\|\phi\|_\varepsilon = \mathcal{O}(\varepsilon^{1/2})$, while $\|u\|_\varepsilon = \mathcal{O}(1)$. Thus for $0 < \varepsilon << 1$, the layer component of the solution is not "seen" by the energy norm and one obtains $\|u\|_\varepsilon \approx \|u\|_0$.

Lin and Stynes [1] address this problem by introducing a new stronger *balanced* norm:

$$\|u\|_\varepsilon = \left\{\varepsilon|u|^2 + \|u\|_0^2\right\}^{1/2}.$$

In this new norm the weighting of the H^1-seminorm has been changed from that of (1). Both of its components, $\varepsilon^{1/2}|u|_1$ and $\|u\|_0$, are now $\mathcal{O}(1)$, and so it is "balanced". Roos and Schopf [4] prove convergence in this norm for a standard Galerkin FEM applied to a singularly perturbed reaction-diffusion problem.

Up to now, no sparse grid method has been analysed in the balanced norm. In this talk we discuss how one can prove convergence in this norm when the two-scale sparse grid method of [2] and the multiscale sparse grid method of [3] are applied to singularly perturbed reaction-diffusion problems. We conclude with numerical experiments.

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Minisymposium M14

Numerical modelling with Freefem++

Organisers

Victorita Dolean and Pierre-Henri Tournier

Solving numerically large scale electromagnetism problems using FreeFem++: high order methods and parallel computing

Marcella Bonazzoli & Victorita Dolean, Ivan G. Graham, Frédéric Hecht, Francesca Rapetti, Euan A. Spence, Pierre-Henri Tournier *(Université Côte d'Azur, France)*

Solving the time-harmonic second order Maxwell's equation is a challenging task because of its indefinite nature and its highly oscillatory solution when the wavenumber is high.

To tackle this problem, we make use of the tools available in FreeFem++ and in its interface with HPDDM, a high-performance unified framework for domain decomposition methods.

In particular, we added to FreeFem++ high order edge finite elements: edge elements are particularly suited to Maxwell's equations and high order methods allow, for a given precision, an important reduction in the number of unknowns and then less computing time.

The resulting discrete system can be ill conditioned, so we couple these high order finite elements with domain decomposition preconditioners. Domain decomposition methods are naturally suited to parallel computing, which becomes necessary to deal with large scale problems.

Finite-element tools for the simulation of Bose-Einstein condensates

Ionut Danaila *(University of Rouen Normandy)*

This is a joint work with F. Hecht, P. Kevrekidis, B. Protas, G. Vergez.

We present several numerical tools using classical finite elements with mesh adaptivity for solving different models used for the study of Bose-Einstein condensates. The programs are written as a toolbox for FreeFem++ (www.freefem.org), a free finite-element software, allowing to easily implement various numerical algorithms [1].

For solving the stationary (imaginary-time) Gross-Pitaevskii equation, we use two robust and optimised numerical methods: a steepest descent method based on Sobolev gradients and a minimization algorithm based on the state-of-the-art optimization library IPOPT. A very recent conjugate-gradient method us-

ing concepts of Riemannian optimization is also presented [2].

For the Bogoliubov-de Gennes system, representing a linearisation of the Gross-Pitaevskii equation, a Newton method and a fast algorithm based on ARPACK for the calculation of eigenvalues are available. For the real-time Gross- Pitaevskii equation, classical splitting and relaxation methods were implemented and intensively tested.

Validations and illustrations are presented for computing difficult configurations with vortices observed in physical experiments: single-line vortex, Abrikosov lattice, giant vortex, dark/anti-dark solitons in one or two-component Bose-Einstein condensates [3].

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Multiphysics and HPC with FreeFem++

Frédéric Hecht & Ionut Danaila, Pierre Jolivet, Frédéric Nataf, Pierre-Henri Tournier *(LJLL, UMPC, Sorbonne Universités)*

FreeFem++ is a powerful and flexible software to solve numerically partial differential equations (PDE) in R^2 and in R^3 with finite elements methods. The FreeFem++ language allows for a quick specification of linear PDEs, with the variational formulation of a linear steady state problem and the user can write their own script to solve non linear problems and time dependent problems. You can solve coupled problems or problems with moving domain or eigenvalue problems, do mesh adaptation, compute error indicators, etc ... This talk will give an overview of the main characteristics of FreeFem++ and demonstrates its application to a range of academic examples.

FreeFem++-js : FreeFem++ with Javascript

Antoine Le Hyaric *CNRS, UMR 7598, Laboratoire Jacques-Louis Lions, France*

FreeFem++ is a computer software implementing a language dedicated to the finite element method. It has already been ported to many hardware computing platforms, but new programming paradigms are emerging and FreeFem++ can take advantage of them. Javascript provides a virtual environment and a language which is an important target because of the omnipresence of the internet. This talk describes how FreeFem++ has been adapted to Javascript. All the new developments required for this transition are listed. The speed of the resulting executable is compared to the previous versions. Several new and interesting ways to use this version of FreeFem++ over the internet are presented, including a new graphical interface and new literate programs.

Microwave tomographic imaging of cerebrovascular accidents by using High-Performance Computing with FreeFem++

Pierre-Henri Tournier *(Université Pierre et Marie Curie)*

Microwave tomography is a novel imaging modality holding great promise for medical applications and in particular for brain stroke diagnosis. From a computational point of view, microwave imaging requires the solution of an inverse problem based on a minimisation algorithm. Reconstruction algorithms are computationally intensive with successive solutions of the electromagnetic forward problem needing efficient numerical modelling and high-performance parallel computing. In this work, we use parallel preconditioners based on Schwarz domain decomposition methods to design fast and robust solvers for the time-harmonic second order Maxwells equation. The efficient parallel implementation of the forward solver as well as the minimisation algorithm in the FreeFem++ framework allows us to demonstrate on synthetic data the feasibility of a microwave imaging technique for the characterisation and monitoring of strokes: we present numerical results for a whole-system modelling of a microwave measurement prototype, where we are able to obtain a tomographic reconstruction of the brain in less than two minutes.

A new stabilised finite element method for a mixed formulation of the convection-diffusion equation

Heather Yorston & Gabriel Barrenechea & Abner Poza *(University of Strathclyde)*

The purpose of this talk is twofold. First, we present a new stabilised finite element method for a mixed formulation of the convection-diffusion equation. This method, a variant of Masud & Kwak's method, has been introduced with the aim of facilitating a new error analysis of this type of method.

As a second step, we compare the new method to a variety of previously existing mixed methods for the convection-diffusion equation in two different standard benchmarks in two space dimensions. Both qualitative and quantitative comparisons are presented. These numerical results confirm the error estimates and show that this present method appears as a competitive alternative to previously existing mixed methods for the CDR equation.

Minisymposium M15

New algorithms related to Chebfun
Organiser
Nick Trefethen

Improvements to the rational Remez algorithm

Silviu Filip & Yuji Nakatsukasa *(University of Oxford)*

Computing rational minimax approximations can be very challenging when there are singularities on or near the interval of approximation — precisely the case where rational functions outperform polynomials by a landslide. We show that far more robust algorithms than previously available can be developed based on adaptive barycentric representations. We describe three algorithms based on this strategy: (1) a "AAA-Lawson" method of iteratively reweighted least-squares, (2) a classical Remez algorithm, and (3) a differential correction algorithm. Our preferred combination, implemented in the Chebfun `minimax` code (superseding the earlier `remez`), is to use (1) in a robust initial phase and then switch to (2) for generically quadratic convergence. By such methods Chebfun can calculate approximations up to type $(80, 80)$ of $|x|$ on $[-1, 1]$ in standard 16-digit floating-point arithmetic in a few seconds, a problem for which Varga, Ruttan, and Carpenter required 200-digit extended precision.

The AAA algorithm for barycentric rational approximation

Yuji Nakatsukasa & Olivier Sète & Lloyd N. Trefethen *(University of Oxford)*

We introduce a new algorithm for approximation by rational functions on a real interval or a set in the complex plane, implementable in 40 lines of MATLAB. Even on a disk or interval the algorithm may outperform existing methods, and on more complicated domains it is especially competitive. The core ideas are (1) representation of the rational approximant in barycentric form with interpolation at certain support points, (2) greedy selection of the support points to avoid exponential instabilities, and (3) least-squares rather than interpolatory formulation of the overall problem. The name AAA, which is pronounced "triple-A", stands for "adaptive Antoulas–Anderson" in honour of the authors who introduced a scheme based on (1).

From random functions to SDEs

Lloyd N. Trefethen & Abdul-Lateef Haji-Ali *(University of Oxford)*

The Chebfun project is about continuous analogues of familiar discrete objects and their realization in Matlab. In Matlab, `randn(n,1)` delivers an n-vector of independent normal $N(0, 1)$ samples. What should the analogous Chebfun command `randnfun` compute? This talk will present the answer we have implemented to that question and its extensions to a rectangle, a box, a sphere, and a disk. Then we turn to questions of Brownian motion, random ODEs, and stochastic DEs. It is an interesting mathematical, scientific, and philosophical question whether noise should be most fruitfully regarded as discrete or continuous.

Minisymposium M16

Networks
Organiser
Francesca Arrigo

Non-backtracking walk centrality for directed networks

Francesca Arrigo, Peter Grindrod, Desmond J. Higham & Vanni Noferini *(University of Strathclyde)*

The talk is motivated by a practical issue: walk-based centrality measures regard all walks of the same length as being equally important, whereas it is intuitively reasonable to rule out certain classes of walk. We focus here on non-backtracking walks. The theory of zeta functions provides an expression for the generating function of non-backtracking walk counts on a directed network. This expression can be used to produce a centrality measure that eliminates backtracking walks at no cost. The new centrality measure may be interpreted as standard Katz on a modified network, where self loops are added, and where non-reciprocated edges are augmented with negative weights. We show that the radius of convergence of the generating function is determined by the spectrum of a three-by-three block matrix involving the original adjacency matrix. This gives a means to choose appropriate values of the attenuation parameter and, in particular, we show that we obtain a larger range of choices for the attenuation parameter than that obtained for standard Katz. By studying the effect of pruning operations on the network (i.e., removing nodes), we show that there is potential for the non-backtracking centrality to be computed more cheaply than Katz for appropriate network structures. Studying the limit as the attenuation parameter approaches its upper bound allows us to propose an eigenvector-based non-backtracking centrality measure in this directed network setting. We illustrate the centrality measure on a synthetic network, where it is shown to eliminate a localization effect present in standard Katz centrality. We also give results for real networks.

Numerical Analysis of Dynamic Centrality

Philip A. Knight *(University of Strathclyde)*

Centrality measures have proven to be a vital tool for analysing static networks. In recent years, many of these measures have been adapted for use on dynamic networks. In particular, spectral measures such as Katz centrality have been extended to take into account time's arrow. We show that great care must be taken in applying such measures due to the inherent ill-conditioning in the associated matrices (an ill-conditioning which can get so extreme that the matrices involved can have a numerical rank of 1). At the same time, the ill-conditioning can reduce computational effort. We investigate some pre-conditioning techniques to alleviate the ill-conditioning, while attempting to keep the costs of computation low.

Centrality Analysis for Modified Lattices

Martin Paton, Desmond J. Higham & Kerem Akartunali *(University of Strathclyde)*

We derive new exact expressions for commonly used network centrality measures, including the Katz and PageRank algorithms, on classical Watts-Strogatz style networks. We are also able to obtain approximations to these vectors that are easy to interpret and highly accurate for large networks. This allows us to compare algorithms and gain insight into the roles of their parameters. We finish by using these techniques to predict behaviour on more complicated examples.

Abstracts of Contributed Talks

Multilevel Solution Algorithms for a Numerical Model of Thin Film Flows

Mashael Al-Johani *(University of Leeds)*

Nonlinear multilevel schemes are well established as fast solvers for nonlinear PDEs of elliptic and parabolic type. In order to find the robust and efficient solution of nonlinear PDE systems, we consider here three nonlinear multilevel schemes which are the Full Approximation Scheme (FAS), Newton-multigrid (Newton-MG) solver and Newton-Krylov solver with a novel preconditioner that we have developed, based upon the use of Algebraic Multigrid (AMG).

We consider the thin film flow as a representative example for the nonlinear system of PDEs. Thin film flow approximations are used in a wide variety of applications from biomedical sciences (e.g. thin tear films in the eye or fluid linings in the lungs of animals) through to engineering and physics (e.g. coating processes in manufacturing or modeling the behavior of a raindrop along a window under the action of gravity). Generally, thin film flows involve a liquid that is bounded between a solid substrate and a free surface with another fluid (frequently air in many applications), the main feature being that the flow is viscous and the motion perpendicular to the substrate may be neglected.

This research studies the robust and efficient solution of a standard thin film flow model. We apply a Finite Difference Method (FDM) in space and a fully implicit scheme in time. At each time step, the resulting discrete nonlinear algebraic system must be solved efficiently. We have developed and contrasted those three nonlinear multilevel schemes to solve this fully discrete system. These schemes are all optimal (i.e. their computational cost grows linearly with the number of degrees of freedom).

In this talk, we will provide a brief summary of the three multilevel solution methods and we will compare their computational performance. We will show theoretical analysis of these schemes, which is providing an insight into how the nonlinear multilevel schemes can be anticipated to perform in practice. Moreover, we will present some numerical results for steady-state and time-dependent problems that demonstrate the optimality of these three approaches, as well as demonstrating, through comparative numerical results, that the best solution strategy of the three is the Newton-Krylov method with our new AMG-based preconditioner.

Solving convection-diffusion and Burgers' equations with random data by stochastic collocation

Eman Almoalim *(University of Manchester)*

PDEs with random data are used to model many phenomena. The aim of this study is to solve the unsteady convection-diffusion equation and Burgers' equation where the diffusion coefficient is a random variable. We use stochastic collocation method to solve the initial boundary value problems numerically and we compare two schemes that are used to solve the deterministic problems. These schemes are the explicit FTCS and the implicit BTCS schemes. We generate the collocation points using Clenshaw-Curtis grid. We study the approximation of statistical quantities (mean and variance) related to the solution of the initial boundary value problems. We also investigate the effects of varying mesh Reynolds number on approximated solution of unsteady convection-diffusion equation where the second norm of the error is used to compare the two schemes. It was found that for mean solution, the FTCS scheme is more accurate than the BTCS scheme while for variance of the solution the error associated with the two methods are very close. For Burgers' equation we consider a discontinuous initial condition. It found that the explicit scheme failed to compute the solution for some cases while the implicit scheme is more effective.

Numerical simulations of a nonlinear Schrödinger model with gain and loss

Z. A. Anastassi & G. Fotopoulos, D. J. Frantzeskakis, T. P. Horikis, N. I. Karachalios, P. G. Kevrekidis, I. G. Stratis, and K. Vetas *(Qatar University)*

We consider the asymptotic behavior of the solutions of a nonlinear Schrödinger (NLS) model incorporating linear and nonlinear gain/loss. We use direct numerical simulations to study the dynamical regimes (depending on the gain/loss strengths), for finite-time collapse, decay, and global existence of solutions in the dynamics [1]-[3].

The model is given by the following equation

$$\begin{aligned} &\mathrm{i}\partial_t u + \frac{1}{2}\partial_x^2 u + |u|^2 u = \mathrm{i}\gamma u + \mathrm{i}\delta |u|^2 u, \\ &x \in \mathbb{R}, \quad t \in [0, T_{\max}). \end{aligned} \tag{1}$$

Here, $u(x,t)$ is the unknown complex field, subscripts denote partial derivatives, and constants $\gamma,\ \delta \in \mathbb{R}$ describe gain or loss. We supplement Eq. (1) with the periodic boundary conditions for u:

$$u(x+2L,t) = u(x,t), \tag{2}$$

for given $L > 0$, and with the initial condition

$$u(x,0) = u_0(x), \tag{3}$$

also satisfying the periodicity conditions (2).

The numerical simulations of some parametric regimes present a special interest, such as the computation of the collapse (blow-up) time. Various techniques have been utilized, including condition of blow-up, variable time-step, high order of discretization of the spatial variable, finite difference methods with various properties (e.g. implicitness, A-stability etc.) and we draw conclusions on their impact in accuracy and efficiency.

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Parallel solver for shifted linear systems with application to model order reduction

Nela Bosner & Zvonimir Bujanović & Zlatko Drmač
(University of Zagreb)

Today, modern developments in science and technology require ever larger dimensional mathematical models. They pose challenging mathematical tasks, that can be tackled using modern numerical methods implemented on state of the art hardware and software tools. Nevertheless, the models may be still too large for numerical simulations, and there is a need for reduction of their dimension. For instance, in case of the LTI dynamical system

$$\dot{x}(t) = Ax(t) + Bu(t),\ \ y(t) = Cx(t)$$

with the system matrix $A \in \mathbb{R}^{n\times n}$ where n can be larger than 10^5, with the input $B \in \mathbb{R}^{n\times m}$, and the output matrix $C \in \mathbb{R}^{p\times n}$, where $m, p \ll n$, one of the approaches is to approximate the system's transfer function

$$\mathcal{G}(s) = C(sI - A)^{-1}B,\ \ s \in \mathbf{i}\mathbb{R}.$$

by a more convenient rational function $\mathcal{G}_r(s)$ of order r with $r \ll n$. One such method is the Iterative Rational Krylov Algorithm (IRKA, S. Gugercin, A.C. Antoulas, and C.A. Beattie., SIMAX 2008), which finds an approximation $\mathcal{G}_r(s)$ that is locally optimal in the norm of the Hardy space $\mathcal{H}_2$. At each iteration, $2r$ shifted linear systems have to be solved in order to obtain the search and the test spaces. Moreover, since IRKA finds only a locally optimal approximation, and in the process of finding an appropriate reduced order model, a user may repeat the computation with different initial shifts (hoping to find better local minimum of the approximation error), and perhaps with several values of r. This design process may, altogether, require solutions of several thousands shifted linear systems.

Even the simple task of graphing the frequency response (Bode plot), i.e. the values of the transfer function $\mathcal{G}(s)$ requires evaluations of $(A - \sigma_j I)^{-1}B$ for many values $\sigma_j = \mathbf{i}\omega_j$, $\omega_j \in \mathbb{R}$. Already for moderately large n, m, p, this mere function evaluation may take an annoyingly long time.

Regardless of hardware capabilities, the problems of middle size are still in focus. In some applications the matrix A is not sparse, and its dimension n is not extremely large, say n is in tens of thousands at most. In such a situation, the total number of shifted systems to be solved, the required accuracy of the solution, and the computing platform (e.g. massively parallel hardware, available optimized libraries) may motivate development of direct methods. In our earlier work, we used *controller Hessenberg form* for efficient solution of a large number of shifted linear systems. The reduction to this form exploits parallel environment very successfully, providing a convenient starting point for the linear solver in the second phase, by reducing number of operations and memory traffic. Shifted linear systems for different shifts are further solved simultaneously. Since modern computers offer execution of numerical algorithms in parallel, performing operations on both CPU and GPU, we adapted this approach to a hybrid CPU+GPU setting. The controller Hessenberg form is computed by splitting the workload between the CPU and the GPU, while the second phase is done entirely on the massively parallel GPU. Besides the efficient BLAS3 operations, we make further use of independent operations that can be carried out simultaneously for different shifts. We

will present our IRKA implementation which is to our best knowledge the first one based on parallel solvers, making it highly parallelizable and efficient.

This work was supported by Croatian Science Foundation grant no. 9345.

Domain decomposition for Navier equations in frequency regime

Romain Brunet & Victorita Dolean *(University of Strathclyde)*

Wave propagation in elastic media is a problem encountered in many fields especially in geophysics. Both experimental and theoretical approaches have been designed because of an increasing interest in man-made ground vibration. Many different methods that have been proposed [4] and have their own range of validity and interest and numerical techniques in the space-time domain can handle any kind of waves in complex media but are limited mainly because of numerical dispersion. For this reason we are interested here in the time-harmonic counterpart of Navier equations with the objective to develop new solvers for this equation which is similar in nature to the Helmholtz and therefore difficult to solve. We will use overlapping domain decomposition methods [2] to split the overall problem into smaller boundary value problems on subdomains and more precisely we will focus on the classic [5] and optimized [1, 3] Schwarz type algorithms. In the first instance we analyse by using the Fourier transform technique, the convergence of these algorithms with the purpose of building more sophisticated methods. Asymptotic results are presented and several numerical results will illustrate the theory.

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Unlocking datasets by calibrating populations of models to data density: a study in atrial electrophysiology

Kevin Burrage & Brodie A. J. Lawson, Christopher C. Drovandi, Nicole Cusimano, Pamela Burrage, Blanca Rodriguez *(Visiting Professor Oxford University and Queensland University of Technology)*

The understanding of complex physical or biological systems nearly always requires a characterisation of the variability that underpins these processes. In addition, the data used to calibrate such models may also often exhibit considerable variability. A recent approach to deal with these issues has been to calibrate populations of models (POMs), that is multiple copies of a single mathematical model but with different parameter values. To date this calibration has been limited to selecting models that produce outputs that fall within the ranges of the dataset, ignoring any trends that might be present in the data.

We present here a novel and general methodology for calibrating POMs to the distributions of a set of measured values in a dataset. We demonstrate the benefits of our technique using a dataset from a cardiac atrial electrophysiology study based on the differences in atrial action potential readings between patients exhibiting sinus rhythm (SR) or chronic atrial fibrillation (cAF) and the Courtemanche-Ramirez-Nattel model for human atrial action potentials.

Our approach accurately captures the variability inherent in the experimental population, allows for uncertainty quantification and also allows us to identify the differences underlying stratified data as well as the effects of drug block.

Backward error of the nonlinear eigenvalue problem expressed in non monomial basis

Hongjia Chen & Tetsuya Sakurai *(University of Tsukuba)*

Given a non-empty open set $\Omega \subseteq \mathbb{C}$, we consider the

nonlinear eigenvalue problem (NEP)

$$F(\lambda)v = 0,$$

where $l \in \Omega \subseteq \mathbb{C}$ and matrix valued-function $F(l) : \Omega \in \mathbb{C}^{n\times n}$.

Instead of solving the NEP $F(\lambda)v = 0$ directly, we compute the eigenpairs of matrix valued-function $R_m(l)$ which is the approximation of $F(l)$, where

$$R_m(l) = b_0(l)D_0 + b_1(l)D_1 + \cdots + b_m(l)D_m,$$

and $D_j \in \mathbb{C}^{n\times n}$ are constant coefficients matrices and $b_j(l)$ are rational or polynomial functions.

To compute eigenpairs of $R_m(l)$, we convert $R_m(l)$ into a linearization form $L(l)$, where

$$L(l) = lA_m + B_m,$$

and $A_m, B_m \in \mathbb{C}^{mn\times mn}$. $L(l)$ and $R_m(l)$ have the same spectrum.

The main motivation of this work is to find a relation between the backward error of eigenpairs of $R_m(l)$ and that of eigenpairs of $L(l)$. To achieve this goal, we construct one-sided factorizations between $L(l)$ and $R_m(l)$. Based on these factorizations, we obtain the bound of the backward error of $R_m(l)$ relative to that of $L(l)$.

CBS constants & their role in error estimation for stochastic Galerkin finite element methods

Adam J. Crowder & Catherine E. Powell *(University of Manchester)*

Forward uncertainty quantification (UQ) is rapidly gaining traction in the physical modelling and engineering communities and stochastic Galerkin finite element methods (SGFEMs) are now commonplace when approximating solutions to PDEs with random or parameter-dependent inputs. However, due to the tensor product structure of the approximation space, it is well known that SGFEMs quickly exhaust desktop computer memory. One technique to reduce the dimension of the approximation space is to initially construct a low-dimensional space, and use a posteriori error estimators to drive its incremental enrichment adaptively. For the enrichment strategy to be effective, the estimators must be accurate. We revisit an error estimator introduced in [A. Bespalov, C.E. Powell, and D. Silvester, Energy norm a posteriori error estimation for parametric operator equations, *SIAM J. Sci. Comput.*, 36(2), 2014] for SGFEM approximations of the parametric diffusion problem. The effectivity of that estimator depends on a CBS (Cauchy-Buniakowskii-Schwarz) constant. If the approximation spaces associated with the parameter domain are orthogonal, then this CBS constant only depends on a pair of finite element spaces, H_1 and H_2 say, on the spatial domain (hence, our results are also applicable to deterministic a posteriori error estimation). For fixed choices of H_1, we investigate various non-standard choices of H_2 and the associated CBS constants, with the aim of designing accurate error estimators (i.e., with effectivity indices close to one). For a model stochastic diffusion problem we demonstrate that very accurate *and* cheap-to-compute estimators are achievable.

Stacked frequency wave inversion for MR elastography

Penny J Davies *(University of Strathclyde)*

Magnetic resonance elastography (MRE) is a rapidly developing field in which the mechanical properties of tissue are reconstructed from MRI shear wave scan measurements. Assuming that the (time-harmonic) tissue displacement is small enough for a linear elasticity model to be valid, then the equation for shear wave propagation in a d-dimensional material is

$$-\alpha^2\,\boldsymbol{u} = \operatorname{div}\left\{\mu\,(\operatorname{grad}\boldsymbol{u} + (\operatorname{grad}\boldsymbol{u})^T)\right\} \quad \text{for } \boldsymbol{x} \in \Omega \subset \mathbb{R}^d, \tag{1}$$

where $\boldsymbol{u} : \Omega \to \mathbb{R}^d$ is the tissue's displacement, $\mu(\boldsymbol{x})$ is an inhomogeneous Lamé material parameter, and α is a nondimensional parameter proportional to the time-harmonic frequency.

Equation (1) is a first order PDE for μ, and the aim is to solve it to reconstruct μ from MRI measurements of $\boldsymbol{u}$. This is obviously impossible from one measurement because there are no boundary conditions for μ. This talk will describe and analyse the new *stacked frequency wave inversion* method in which multi-frequency information is used to obtain a robust reconstruction algorithm. It is joint work with Eric Barnhill and colleagues at the Charité Universitätsmedizin, Berlin.

Accurate and fast algorithms for some subclasses of totally positive matrices

Jorge Delgado & Juan Manuel Peña *(Universidad de Zaragoza)*

An algorithm using only products, quotients, additions of numbers with the same sign or subtractions of initial data provides a result computed to high relative accuracy (HRA) (cf. [5, 6]). In this talk we will present HRA algorithms for some problems in numerical linear algebra (linear system solving, eigenvalue computation, singular value computation and inverse computation) for some subclasses of totally positive (TP) matrices arising in several fields: Computer Aided Geometric Design (cf. [7, 1, 3]), Financial applications (cf. [4]), Combinatorics (cf. [2]), ... In addition to explicit algorithms, we will provide insights of the different techniques used to obtain them.

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Exponential convergence in $H^{1/2}$ of hp-approximation for parabolic equations

Denis Devaud & Christoph Schwab *(ETH Zürich)*

We discuss and analyze a continuous hp-finite element approximation (FEM) for linear parabolic evolution problems considering a novel framework due to Fontes [2]. This space-time formulation is based on Sobolev spaces of fractional order for the time variable, yielding a weak form containing fractional derivatives. These spaces as well as some of their properties and equivalent characterizations are first presented. We then define an isomorphism which allows us to show explicitly that the bilinear form associated to the weak formulation of the problem is inf-sup stable. This is a big advantage when considering a FEM approximation of the parabolic equations since we can then build arbitrary inf-sup stable pairs of discrete spaces. To the authors' knowledge, we are the first ones to consider such a framework in the context of numerical analysis.

Using the best approximation property of the discrete solution, we need to define an interpolation operator and derive associated a priori error estimates. Hence, based on an idea from Babuška and Guo [3], we define such an operator and present bounds in the L^2- and $H^{1/2}$-norms which are fully explicit in the mesh-width and the polynomial degree. This gives convergence rates for standard h- and p-FEM approximations assuming that the solution is smooth enough. However, solutions of parabolic equations are typically smoothened over time but contain an algebraic singularity at the initial time due to a mismatch between the right-hand side and the initial condition. In particular, they belong to a certain class of Gevrey functions. Using graded meshes and increasing polynomial degrees, we present one of our main results which shows that it is possible to obtain exponential convergence for such functions.

We discuss further a specific instance of this theory, namely the two dimensional heat equation. In particular, we state that exponential convergence can be obtained also when the solution contains singularities in the space variable. We conclude the presentation by showing numerical results in accordance with the developed theory.

Complete proofs of all the results presented in this talk can be found in [1].

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Efficient approximation of the 2nd order acoustic wave equation

Dugald B Duncan *(Heriot-Watt University)*

The 2nd order acoustic wave equation in an isotropic homogeneous medium can be written as $u_{tt} = \Delta u$ and is of course coupled with appropriate initial and boundary conditions. There are many good schemes for solving this equation and its inhomogeneous generalisation. Cohen's book explains the spectral element method (SEM). The SEM uses a Galerkin finite element method in space with higher order elements used for higher accuracy schemes, coupled with mass-lumping (hence explicit time-stepping) and a modified equations approach to achieving higher-order time accuracy – essentially a finite difference methodology in time. These schemes work well and are highly competitive for efficiency on irregular grids. In this talk we examine the relationship between these general-grid SEM methods, and some more efficient schemes with related structures that can be derived on uniform grids (in more than 1 space dimension). We then examine how these two approaches can be blended.

'Exact' finite difference scheme to single-compartment pharmacokinetic models

Oluwaseun Francis Egbelowo, Charis Harley & Byron A. Jacobs *(University of the Witwatersrand)*

The motivation for this study was to provide a non-standard finite difference (NSFD) scheme to one-compartment pharmacokinetics models. These models comprise of linear and nonlinear ordinary differential equations. 'Exact' finite difference schemes were provided for the linear models while we applied the NSFD rules based on Mickens' idea to transform the nonlinear models into the discrete schemes. The method was compared with established methods to verify the efficiency and the accuracy of the method. A simulation study of the one-compartment pharmacokinetic model with different routes of administration was made.

Convergence of a Semi-Discrete Numerical Method for a Class of Nonlocal Nonlinear Wave Equations

H. A. Erbay *(Ozyegin University, Turkey)* & S. Erbay *(Ozyegin University)* & A. Erkip *(Sabanci University)*

In this study, we prove the convergence of a semi-discrete numerical method applied to a general class of nonlocal nonlinear wave equations where the nonlocality is introduced through the convolution operator in space. The most important characteristic of the numerical method is that it is directly applied to the nonlocal equation by introducing the discrete convolution operator. Starting from the continuous Cauchy problem defined on the real line, we first construct the discrete Cauchy problem on a uniform grid of the real line. Thus the semi-discretization in space of the continuous problem gives rise to an infinite system of ordinary differential equations in time. We show that the initial-value problem for this system is well-posed. We prove that solutions of the discrete problem converge uniformly to those of the continuous one as the mesh size goes to zero and that they are second-order convergent in space. We then consider a truncation of the infinite domain to a finite one. We prove that the solution of the truncated problem approximates the solution of the continuous problem when the truncated domain is sufficiently large. Finally, we present some numerical experiments that confirm numerically both the expected convergence rate of the semi-discrete scheme and the ability of the method to capture finite-time blow-up of solutions for various convolution kernels.

Foundations and Numerics of the Maxwell-LLG equations

Michael Feischl & Thanh Tran *(UNSW Sydney)*

We analyze a numerical method for the coupled system of the eddy current equations in three space dimensions with the Landau-Lifshitz-Gilbert equation in a bounded domain. The unbounded domain is discretized by means of finite-element/boundary-element coupling. Even though the considered problem is strongly nonlinear, the numerical approach is constructed such that only two linear systems per time step have to be solved. We prove unconditional weak convergence (of a subsequence) of the finite-element solutions towards a weak solution. We establish a priori error estimates if a sufficiently smooth strong solution exists.

Rank deficiency and nearness to Krylov subspaces in finite-precision computations

Tomáš Gergelits & Marie Kubínová, Iveta

Hnětynková *(Charles University, Prague)*

Krylov subspace methods represent a computationally attractive way of solving large and sparse linear algebraic problems

$$Ax = b, \qquad A \in R^{n\times n}, \quad b \in R^n.$$

Many of them rely mathematically on computing an orthonormal basis of the Krylov subspaces

$$\mathcal{K}_k(A, r_0) \equiv \text{span}\{r_0, Ar_0, \ldots, A^{k-1}r_0\}, \quad k = 1, 2, \ldots.$$

For a symmetric matrix, a sequence of the basis vectors can be computed by short recurrences, in particular by the Lanczos tridiagonalization.

Due to the effect of rounding errors, however, the use of short recurrences in practical computations inevitably leads to the loss of global orthogonality and even to the loss of linear independence among the generated vectors. Consequently, the generated susbpaces become rank-deficient, which may cause a significant delay of convergence. Thus, the structure of Krylov subspace methods as an optimal projection process onto nested subspaces of increasing dimensionality seems to be lost.

In this contribution, we investigate whether, in which sense, and how accurately, the first k steps of the finite precision arithmetic computation can be related to the first l steps of the exact computation with the same matrix and the starting vector. This allows us to compare not only the convergence curves, but also the computed approximations or the corresponding residuals. Moreover, we can study the nearness of the generated subspaces with exact Krylov subspaces.

Linearly Convergent Randomized Iterative Methods for Computing the Pseudoinverse

Robert M. Gower *(Inria - ENS)* & Peter Richtárik *(University of Edinburgh)*

We develop the first stochastic incremental method for calculating the Moore-Penrose pseudoinverse of a real matrix. By leveraging three alternative characterizations of pseudoinverse matrices, we design three methods for calculating the pseudoinverse: two general purpose methods and one specialized to symmetric matrices. The two general purpose methods are proven to converge linearly to the pseudoinverse of any given matrix. For calculating the pseudoinverse of full rank matrices we present two additional specialized methods which enjoy a faster convergence rate than the general purpose methods. We also indicate how to develop randomized methods for calculating approximate range space projections, a much needed tool in inexact Newton type methods or quadratic solvers when linear constraints are present. Finally, we present numerical experiments of our general purpose methods for calculating pseudoinverses and show that our methods greatly outperform the Newton-Schulz method on large dimensional matrices.

Mathematical modelling and numerical results for bioglasses

A. Hadji & M.L. Hadji
(Mathematical Modelling and Numerical Simulation Laboratory & LAPS, Badji Mokhtar University)

In this work we develop a mathematical model for glass materials using thermal properties. These substances are porous bioactive materials that can be suitable for many applications such as prolonged-release drug or bone tissue repairing. To detect the chemical modifications induced by modifying the Ca/P molar ratio, we first derive a new system of differential equations, by taking into account additional terms, due to the concentration inhomogeneities of the used compounds. Then we propose a numerical approach to solve our system in order to illustrate the behaviour and the dynamics of the chemical bonding, structural and morphological properties of the resulting amorphous glass process. At this stage, we start by showing a stability result for our numerical scheme and then present numerical results.

Keywords: Bioglass, Modelling, Finite elements, Stability Analysis.

On the order of convergence of AMF-W-methods for the time integration of parabolic PDEs

S. González-Pinto, **D. Hernández-Abreu**, S. Pérez-Rodríguez *(University of La Laguna)*

This talk deals with families of W-methods equipped with the splitting provided by the Approximate Matrix Factorization (AMF). The so-called AMF-W-methods have proved to be an efficient alternative when solving large systems of ODEs coming from the spatial discretization of time-dependent PDEs (in 2 or 3 spatial dimensions) by means of finite differences or finite volumes.

We are mainly focussed on the analysis of the order

reduction phenomenon suffered by the methods when time dependent Dirichlet boundary conditions are imposed. This will be carried out by considering 2D and 3D standard linear parabolic PDEs with a time dependent reaction source and no errors in the spatial discretization.

The orders of convergence (both in ODE and PDE sense) of some relevant AMF-W-methods considered in the literature [1-3,5] for the time integration of parabolic PDEs are described. In particular, we consider an AMF-W-method whose underlying explicit Runge-Kutta method equals the classical Kutta's 3/8-Rule, whereas the remaining coefficients have been optimized for stability purposes [1] and high order of convergence on index-1 DAEs [4]. As a matter of fact, the newly proposed AMF-W-method turns to be A-stable as a ROW method (Rosenbrock-Wanner method) and it has order four (as ROW method) and order three as W-method for both ODEs and DAEs of index one. Some details about the implementations of the methods are also provided.

Finally, a boundary correction technique is proposed in order to recover the convergence order as if time-independent boundary conditions were imposed.

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Tropically linear regression and low rank matrix approximation

James Hook *(University of Bath)*

Tropical algebra concerns any semiring whose 'addition' operation is max or min. In my talk I will focus on the max-plus semiring $\mathbb{R}_{\max} = [\mathbb{R} \cup \{-\infty\}, \oplus, \otimes]$, with $a \oplus b = \max\{a, b\}$ and $a \otimes b = a + b$, for all $a, b \in \mathbb{R}_{\max}$. Tropical algebra has the potential to describe certain classically non-linear phenomena in a linear way. For example many queuing models turn out to be linear over $\mathbb{R}_{\max}$. Similarly many discrete optimizations problems including shortest paths problems have a tropically linear structure.

When dealing with datasets from such applications it is natural to ask whether tropical analogues of classical linear algebra approaches will be effective. To this end I will discuss using max-plus linear regression to analyze time series data recorded from a queuing system and using max-plus low rank approximate matrix factorization to reveal structure in large networks.

Numerical simulation of pure diffusion and reaction diffusion models by Haar wavelets

Siraj-ul-Islam & Muhammad Ahsan& Imran Aziz *(University of Engineering and Technology Peshawar)*

In this work, we present a new method for solving Elliptic PDEs (EPDEs), Pure Diffusion Model (PDM) and Reaction Diffusion Model (RDM) by using Haar wavelets.

The new work is the extension and improved form of the earlier work based on Haar wavelet methods [1]. In this paper the earlier algorithm [1] has been modified by starting the approximation with the fourth mixed derivative rather than the second derivatives w. r. t. x and y separately. The methods are then vectorized using the Kronecker tensor product. Consequently, the efficiency of the earlier algorithms [1] has been enhanced manyfold. We have also introduced some structural changes which make the methods applicable to more general classes of PDEs containing mixed derivatives as well. Like the earlier case [1], the time derivative is replaced by the Euler formula. The Haar wavelets approximation combined with the Euler formula reduce the governing differential equations along with given boundary and initial conditions into a system of algebraic equations. Numerical results thus obtained are compared with analytical solutions as well as other numerical methods. A distinctive feature of the proposed method is its simple applicability for a variety of boundary conditions. The efficiency of the method is demonstrated by five different benchmark

tests.

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Accurate eigenvalue decomposition of rank-one modifications of diagonal matrices

Nevena Jakovčević Stor & Ivan Slapničar & Jesse L. Barlow *(University of Split)*

We present an algorithm for solving an eigenvalue problem for a real symmetric matrix which is a rank-one modification of a diagonal matrix. The algorithm computes each eigenvalue and all components of the corresponding eigenvector with high relative accuracy in $O(n)$ operations. The algorithm is based on a shift-and-invert approach. Only a single element of the inverse of the shifted matrix eventually needs to be computed with double the working precision.

Each eigenvalue and the corresponding eigenvector can be computed separately, which makes the algorithm adaptable for parallel computing.

An Optimization Based Multilevel Algorithm for Selective Variational Image Segmentation Models

Abdul K. Jumaat & Ke Chen *(Center for Mathematical Imaging Techniques and University of Liverpool)*

Variational active contour models have become very popular in recent years, especially global variational models which segment all objects in an image. Given a set of user-defined prior points, selective variational models aim to segment selectively one object only. We are concerned with fast solution of the latter models. Time marching methods with semi-implicit schemes and an additive operator splitting method are used frequently to solve the resulting Euler Lagrange equations derived from these models. For images of moderate size, such methods are effective. However, to process images of large size, urgent need exists in developing fast iterative solvers. Here we propose an optimization based multilevel algorithm for efficiently solving a class of selective segmentation models. In level set function formulation, our first variant of the proposed multilevel algorithm has the expected optimal $O(N \log N)$ efficiency for an image of size $n \times n$ with $N = n^2$. However modified localized models are proposed to exploit the local nature of segmentation contours and consequently our second variant after further acceleration is up to practically super-optimal efficiency $O(\sqrt{N} \log N)$. Numerical results show that good segmentation quality is obtained and as expected excellent efficiency observed in reducing computational time.

A New MITC Finite Element Method for Reissner-Mindlin Plate Equations Using a Bi-orthogonal System

Bishnu Lamichhane & Mike Meylan *(University of Newcastle, Australia)*

We present a new MITC (Mixed Interpolated Tensorial Components) finite element method for Reissner–Mindlin plate equations. The new finite element method uses a biorthogonal system to construct the reduction operator for the MITC element. Numerical results are shown to demonstrate the performance of the approach.

High order DGFEM in time for linear wave equations

Matthias Maischak & Fatima Al-Shanfari *(Brunel University)*

We analyse a high order discontinuous Galerkin finite element method (DGFEM) in time for abstract linear wave equations. Our approach is based on re-writing the 2nd order wave equation as a first order system, as done by C. Johnson (1993) for the acoustic wave equation with linear functions in time and then apply the high order discontinuous Galerkin discretization as done by D. Schötzau (1999) for parabolic problems. The resulting first order system is not parabolic, i.e. standard arguments don't apply. In particular the underlying space dependent bilinear form in the first order system is not symmetric and positive definite, but skew-symmetric and fullfills the inf-sup condition only in a non-conformal combination of energy norm and Hilbert spaces. We have shown solvability, stability and a priori estimates for the system in abstract Hilbert spaces. Our approach allows parallelisation in the time-stepping procedure and large time-steps. We also apply our approach to a problems with non-homogeneous Dirichlet boundary data, in particular the acoustic and elastic wave equations and scatter-

ing problems.

Two improved iteration methods for the nonlinear matrix equation $X = R+M^T(X^{-1}+B)^{-1}M$

Jie Meng & Hyun-Min Kim *(Pusan National University)*

In this talk, we consider the nonlinear matrix equation $X = R+M^T(X^{-1}+B)^{-1}M$, where M is an arbitrary $n\times n$ real matrix, and R and B are symmetric positive semidefinite matrices. Note that this matrix equation is the well-known discrete algebraic Riccati equation (DARE), and for obtaining its positive definite solution, we propose one inversion-free variant iteration method and a new quadratically convergent iteration method by applying the cyclic reduction. Finally, we give some numerical examples to show the efficiency of the proposed iteration methods.

A sharp maximum principle for a two-point boundary value problem with a Caputo fractional derivative

Xiangyun Meng & Martin Stynes *(Beijing Computational Science Research Center)*

The analysis of finite difference methods often depends on discrete maximum principles. One can expect a difference scheme to have this property only if the boundary value problem that it approximates satisfies a continuous maximum principle. Thus it is of interest to investigate when fractional-derivative boundary value problems satisfy maximum principles—this is a non-trivial question in general. For the Caputo two-point boundary value problem that we will consider, example [2, Example 2.1] shows that, unlike the classical elliptic case, Dirichlet boundary conditions won't guarantee a maximum principle. What boundary conditions will yield a maximum principle? To the best of our knowledge, only one maximum principle result [1] is known for this Caputo problem, and it is easy to see that this result is not sharp. We derive an explicit formula for the Green's function of our boundary value problem. After some analysis of this Green's function we obtain a sharp maximum principle.

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About the extension of the DPG method to Banach spaces

Ignacio Muga[1] & Kristoffer G. van der Zee[2] *(1: Pontifical Catholic University of Valparaíso, Chile; 2: The University of Nottingham)*

In this talk we analyze the main aspects about extending the DPG method to a Banach space setting.

The *Discontinuous Petrov-Galerkin* (DPG) method proposed by Demkowicz & Gopalakrishnan [1] has captured the attention of numerical analysts in this decade. The method computes problem-dependent *optimal test functions* in order to guarantee discrete stability. The last becomes computationally attractive only when the variational formulation makes use of discontinuous or *broken* Sobolev test spaces.

The DPG method relies on some Hilbert space features as the inner product and the *Riesz representation map*. This prevents us from a straightforward extension of the method to a Banach space setting. However, as it is shown in [1], the DPG method can be seen as residual minimization method in a dual norm. We exploit this idea as the starting point to develop a method suitable for Banach spaces. As a result we derive a non-linear monotone mixed Petrov-Galerkin method [2] which recovers the DPG method for Hilbert space settings. We show the well-posedness of this method, together with error estimates, and some basic numerical experiments in 1D.

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Stable computation of the matrix functions $\cosh\sqrt{A}$ and $\operatorname{sinhc}\sqrt{A}$

Prashanth Nadukandi & Nicholas J. Higham

(University of Manchester)

We present a backward stable algorithm for computing $\cosh\sqrt{A}$ and a mixed stable algorithm for computing $\mathrm{sinhc}\sqrt{A}$. Our new algorithms employ Padé approximant of $\cosh\sqrt{x}$ combined with scaling and use of a double angle formula. The backward error of this approximation is expressed as a hypergeometric function. The rational approximant for $\mathrm{sinhc}\sqrt{x}$ and the associated mixed approximation error are obtained by taking the derivative of the Padé approximant of $\cosh\sqrt{x}$ and its backward error. The amount of scaling and the degree of the approximants are chosen to minimize the computational cost subjected to backward stability in exact arithmetic.

Condition numbers for Yang-Baxter matrix equation

Syed Muhammad Raza Shah Naqvi & Hyun-min Kim *(Pusan National University)*

In this talk, we consider the three types of condition numbers, i.e Normwise, Componentwise and Mixed, for the Yanf-Baxter matrix equation(independently introduced by C.N. Yang in 1968 and T.R. Baxter in 1971 in statistical mechanics) and derived their explicit expressions. We give some numerical examples to show the efficiency and difference between the proposed condition numbers.

An efficient reduced basis method for the stochastic groundwater flow problem

Craig J. Newsum & Catherine E. Powell *(University of Manchester)*

Reduced basis methods (RBMs) allow us to reduce the computational cost associated with solving parameter dependent PDEs which arise in *uncertainty quantification* (UQ) where, in particular, many choices of parameters need to be considered. Constructing a reduced basis involves a computationally demanding offline stage, which is performed only once, but allows us to cheaply approximate the parameter dependent PDE online for many choices of parameters.

In this talk, we develop an *efficient* RBM for the parameter dependent saddle point problem arising from the mixed formulation of the Darcy flow problem in groundwater flow modelling with *uncertain* coefficients. We approximate the diffusion coefficient using the discrete empirical interpolation method and combine the RBM with a sparse grid stochastic collocation mixed finite element method to construct a surrogate solution which then allows for efficient forward UQ. We present numerical results from [1] that demonstrate the significant reduction in computational cost achieved using our scheme over standard high fidelity methods.

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Elliptical contour based inversion of Laplace transform and application to Black&Scholes and Heston equations

Giancarlo Nino *(Gran Sasso Science Institute)* & Nicola Guglielmi *(University of L'Aquila)*

The inverse Laplace transform is a powerful tool that has been employed in several numerical problems. In particular, let us consider a linear parabolic differential equation of the form

$$\frac{\partial u}{\partial t} = \mathcal{A}(u), \qquad \text{with } \mathcal{B}(u) = 0, \tag{1}$$

where $\mathcal{A}$ involves u and its spatial derivatives and $\mathcal{B}(u)$ indicates some boundary condition. If we discretize in space (1), we get the following Cauchy problem

$$u'(t) = Au(t) + b(t), \qquad u(0) = u_0. \tag{2}$$

Applying Laplace transform $\mathcal{L}$ to both sides of (2), we get an algebraic equation for $\hat{u} = \mathcal{L}(u)$. Using the well known Bromwich inversion formula, we obtain

$$u(t) = \frac{1}{2\pi i}\int_\Gamma e^{zt}\hat{u}(z)\,dz \tag{3}$$

where Γ is a suitable contour in the complex plane. In the last years, great attention to the method has been paid, due to the application to some numerically challenging PDEs. In particular, in [1], [2] hyperbolic contours are used and an exponential convergence is reached. In [3], the author proposes a method based on parabolic contours, still getting an exponentially convergent scheme. Motivated by the recent works [1, 2, 4], we propose a new inversion technique that is based on the integration over open arcs of ellipse. Once the time is fixed, the choice of the integration contour is guided by the computation of the pseudospectral level curves of the discrete operator A. The method is exponentially convergent and stable. Numerical examples on Black&Scholes and Heston equations are provided. The comparison with the other cited methods shows that the method is competitive.

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Dynamical behaviour of miscibles fluids in Porous Media

F.Z. Nouri, A. Assala & N. Djedaidi
(Badji Mokhtar University)

In this work, we are interested in studying the dynamics of miscible fluids in porous media. The model describing this issue is a system of equations, coupling the standard Navier-Stokes equations with gravity g as external force and a convective diffusion equation for a dilute concentration in the carrier fluid. By assuming that the fluids are incompressible, we first derive a new system of equations, by taking into account additional terms, due to the concentration inhomogeneities and an interfacial tension between the fluids. Then we propose a numerical approach to solve our system in order to illustrate the effectiveness of the dynamics during the fluid miscibility process. At this stage, we start by showing a stability result for our numerical scheme and then present numerical results.

Keywords: Fluid Dynamics, Finite Elements, Stability, Porous media.

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Approximating Coupled Hyperbolic-Parabolic Systems Arising in Enhanced Drug Delivery

José A. Ferreira & Daniela Jordão & **Luís Pinto**
(University of Coimbra)

In this talk we consider a system of partial differential equations defined by a hyperbolic equation and a parabolic equation. The convective term of the parabolic equation depends on the solution and eventually on the gradient of the solution of the hyperbolic equation. This system arises in the mathematical modeling of several physical processes as for instance ultrasound enhanced drug delivery. In this case the propagation of the acoustic wave, which is described by a hyperbolic equation, induces an active drug transport that depends on the acoustic pressure. Consequently the drug diffusion process is governed by a hyperbolic and a convection-diffusion equation.

We propose a numerical method that allows us to compute second order accurate approximations to the solution of the hyperbolic and the parabolic equation. The method can be seen as a fully discrete piecewise linear finite element method or as a finite difference method. The convergence rates for both approximations are unexpected. In fact we prove that the error for the approximation of the pressure and concentration is of second order with respect to discrete versions of the H^1-norm and L^2-norm, respectively.

Numerical examples illustrating the theoretical results and an application to enhanced drug delivery are also presented.

Derivative-Free Optimisation Methods for Non-

linear Least-Squares Problems

Lindon Roberts & Coralia Cartis *(University of Oxford)*

Derivative-free optimisation (DFO) algorithms are a category of optimisation methods for situations when one is unable to compute or estimate derivatives of the objective. The need for DFO arises in applications where techniques such as finite differencing or algorithmic differentiation are inaccurate or impractical, such as when the objective has noise (e.g. Monte Carlo simulations in finance) or is very expensive (e.g. climate simulations).

In this talk I will present a flexible derivative-free Gauss-Newton framework for unconstrained nonlinear least-squares problems. This framework is a simplification and improvement over state-of-the-art model-based trust region DFO methods for nonlinear least-squares [Zhang, Conn & Scheinberg, SIAM J. Optim., 20 (2010), 3555-3576]. Time permitting, I will discuss particular features of this framework, such as a low initialisation cost (in terms of objective evaluations) and improved performance for stochastic problems.

An adaptive stochastic Galerkin FEM for parametric PDEs with singular solutions

Leonardo Rocchi & Alex Bespalov *(University of Birmingham)*

We consider elliptic PDE problems with random coefficients that have affine dependence on a large, possibly infinite, number of random parameters. For example, the coefficients given in terms of polynomial chaos or Karhunen-Lòeve expansions can be considered. Discretisations of such problems can be obtained by using stochastic Galerkin Finite Element Methods (sGFEMs). They generate approximations of the solution in tensor product spaces $X \otimes P$, where X is a finite element space associated with a spatial domain $D \subset \mathbb{R}^2$ and P is a finite-dimensional space of multivariate polynomials in the parameters.

The adaptive algorithm proposed in [A. Bespalov and D. Silvester, SIAM J. Sci. Comput., 38(4): A2118–2140, 2016] employs a hierarchical a posteriori error estimation strategy which leads to distinct estimators associated with two sources of discretisation error. At the same time, such estimators provide effective estimates of the error reduction that will occur if different enhanced approximations are computed. In particular, the enrichment of the finite element space is based on uniform refinements of the spatial mesh, allowing an efficient discretisation of spatially regular problems. We have recently extended the above algorithm in order to deal with problems having spatially singular solutions. At each iteration, either a local refinement of the underlying triangulation or a polynomial enrichment on the parameter domain is pursued. To this end, we employ Dörfler marking for both spatial and parametric approximations, and enhance the approximation corresponding to the larger estimate of the error reduction.

In this talk, we will describe the developed adaptive algorithm and demonstrate its performance for two elliptic model problems with random coefficients posed over an L-shaped and a crack domain. In particular, we will show how the local mesh refinement works appropriately with respect to both spatial singularities in the mean value and in the variance of the solution. For each model problem, the convergence of the algorithm will be demonstrated numerically.

Solving integral equations for electromagnetic scattering using BEM++

Matthew Scroggs & Timo Betcke & Erik Burman & Wojciech Śmigaj & Elwin van 't Wout *(University College London)*

The numerical simulation of electromagnetic wave scattering poses significant theoretical and computational challenges. Much effort in recent years has gone into the development of fast and robust boundary integral equation formulations to simulate a range of phenomena from the design and performance of antennas to radar scattering from large metallic objects.

While there have been a range of important theoretical advances in recent years for the development of robust preconditioned boundary integral formulations for Maxwell, the computational implementation remains a challenge. At University College London, as part of the BEM++ project, we have developed a number of easy to use Python-based open-source tools to explore and solve Maxwell problems based on preconditioned electric field (EFIE), magnetic field (MFIE) and combined field (CFIE) integral equation formulations.

In this talk, we will give an overview of these formulations using an example exterior wave scattering problem. We will look at the importance of carefully selecting the finite dimensional spaces in order to pro-

duce a stable discretisation of the formulations, and compare the formulations using a number of interesting, non-trivial domains.

A walk-outside-spheres for the fractional Laplacian

Tony Shardlow & Andreas Kyprianou *(Bath)* & Ana Osojnik *(Oxford)*

By using the Feynman–Kac formula for an α-stable Levy process, we derive an unbiased method for solving the fractional Laplace equation on a domain with exterior Dirichlet data. The method is motivated by the classical walk-on-spheres algorithm for the boundary-value problem for the Laplacian.

Flexible and deflated variants of the block shifted GMRES method

Dong-Lin Sun & Ting-Zhu Huang & Bruno Carpentieri & Yan-Fei Jing *(UESTC,Rug)*

We consider the iterative solution by preconditioned Krylov subspace methods of sequences of shifted linear systems with L shifts and p different right-hand sides given at once of the form

$$(A - \sigma_i I)X_i = B, \text{ with } i = 1, 2, \ldots, L,$$

where the scalars $\{\sigma_i\}_{i=1}^{L} \subset \mathbb{C}$ are called shifts, $A - \sigma_i I \in \mathbb{C}^{n\times n}$ are large square nonsingular matrices of dimension n, I is the identity matrix of order n, and $B = [b^{(1)}, b^{(2)}, \ldots, b^{(p)}]$ is the $n \times p$ right-hand sides matrix. We assume that B is a full rank matrix. The problem arises, e.g., in the solution of lattice quantum chromodynamics problems, Tikhonov-Philips regularization, Newton trust region optimization and PageRank computation.

We propose a new flexible and deflated shifted block GMRES method that solves the whole sequence of multi-shifted linear systems simultaneously, detecting effectively the linear systems convergence, and allows us to use variable preconditioning. We present the main lines of development of the new Krylov method, describe its theoretical properties, and illustrate several numerical experiments showing its good performance against other block and non-block shifted iterative techniques for solving general sparse linear systems as well as in PageRank calculations.

Numerical methods for the fractional diffusion equation

Béla Szekeres & Ferenc Izsák *(MTA-ELTE, Budapest)*

In this talk we review and analyze the Matrix Transformation Method for the efficient solution of the fractional diffusion equation.

The accurate measurement techniques of the last decade confirmed the presence of the fractional diffusion in many phenomena in the natural sciences. A suitable mathematical model of this dynamic can be obtained by the following equation:

$$\begin{cases} \partial_t u(t,x) = -\mu \left(-\Delta\right)^{\alpha/2} u(t,x), & t > 0,\ x \in \mathbb{R}^n \\ u(0,x) = u_0(x), & x \in \mathbb{R}^n, \end{cases} \tag{1}$$

where a possible choice for the differential operator is

$$\begin{aligned} &\Delta^{\alpha/2} = -\left(-\Delta\right)^{\alpha/2} f(x) \\ &:= \frac{C(n,\alpha/2)}{2} \int_{\mathbb{R}^n} \frac{f(x+y) + f(x-y) - 2f(x)}{|y|^{n+\alpha}}\, \mathrm{dy}, \end{aligned}$$

with $C(n,\alpha/2)$ a special constant and $\mu > 0$ a given coefficient.

To model real-life phenomena, we should restrict (1) to a bounded domain $\Omega \subset \mathbb{R}^n$ and define an appropriate fractional Laplacian operator $\Delta^{\alpha/2}$. We pointed out that among the possible definitions for $\Delta^{\alpha/2}$, the spectral approach seems to be the only suitable one [2].

For the corresponding numerical approximations there were two ways proposed in the multidimensional case. The first one, which works with a dimensional extension is discussed in [3] and [4]. Another way, which we followed is based on the discrete version of the spectral decomposition, the *matrix transformation technique* (MTM) [1].

The main idea of the MTM is the following: if (with some discretization) A_h approximates the operator $-\Delta$, then $A_h^{\alpha/2}$ gives an approximation of the operator $(-\Delta)^{\alpha/2}$.

In [5], we proved the quasioptimality of the MTM in the L_2-norm for the corresponding elliptic problems for the FE approximation. We also proved in this case that the MTM combined with FD approximation gives an optimal error bound [6].

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Shape Optimization with Geometric Constraints Using Moreau-Yosida Regularization

Florian Wechsung & Patrick Farrell *(University of Oxford)*

Shape optimization has received significant interest from both a theoretical and an applied point of view over the last decades. The approaches used can roughly be categorized into those based on using a parametrization for the shape or its deformation and then applying an optimization algorithm to the discretized problem (discretize-then-optimize) and those that formulate the problem as optimization over an infinite-dimensional space of shapes or deformations and then discretize afterwards (optimize-then-discretize). We follow the latter approach and search for diffeomorphisms $T \in [W^{1,\infty}(\Omega)]^d$ that deform an initial shape Ω. The optimization problem then reads as follows

$$\underset{T \in \mathcal{X} \cap K}{\text{minimize}} \quad J(T(\Omega)).$$

We choose $\mathcal{X} = \{T \in [W^{1,\infty}(\Omega)]^d : T \text{ is a } W^{1,\infty}\text{-diffeomorphism}\}$ as the space of admissible deformations as Lipschitz regularity of the domain is needed by many problems in which a PDE constraint is included in the optimization problem.

Furthermore we want to include certain geometric constraints; this is represented by the requirement $T \in K$. A classical example for a geometric constraint that is often considered is volume/mass conservation, i.e. $K = \{T \in \mathcal{X} : \text{vol}(T(\Omega)) = \text{vol}(\Omega)\}$. In our work we investigate constraints of the form

$$K = \{T \in \mathcal{X} : T(\partial\Omega) \subset C\}$$

for some convex set $C \in \mathbb{R}^d$. A classical application where this is relevant is wing design in Formula 1, where the teams are given bounding boxes in which the wing needs to be contained.

To include this constraint, we begin by considering the indicator function $\phi : L^2(\partial\Omega) \to (-\infty, +\infty]$, defined via

$$\phi(T) = \begin{cases} 0, & \text{if } T(\partial\Omega) \subset C \\ +\infty, & \text{otherwise,} \end{cases}$$

and observe that (1) is equivalent to

$$\underset{T \in \mathcal{X}}{\text{minimize}} \quad J(T(\Omega)) + \phi(T).$$

Classically the Moreau-Yosida regularization of ϕ is then used to implement path-following methods; in the context of shape optimization this has been done in [1]. However, in [2] it was shown that the Moreau-Yosida regularization of ϕ can also be used to formulate augmented Lagrangians. We adapt the latter approach to the case of PDE constrained shape optimization and present numerical examples implemented in the `Firedrake` finite element software.

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A Gauss-Hermite Quadrature Method for the Inversion of the Laplace Transform

J.A.C. Weideman *(Stellenbosch University)*

Many numerical inversion methods for the Laplace transform approximate the complex contour integral formula known as the Bromwich integral. This approach has two key ingredients: (a) a choice of quadrature rule, and (b) a choice of contour. The latter choice is a freedom offered by Cauchy's theorem, which

allows one to deform the original Bromwich line (parallel to the imaginary axis) to a contour that has better properties for numerical computation.

One of the most popular methods in this class is Talbot's method. It uses (a) the trapezoidal rule, on (b) a cotangent contour that begins and ends in the left half-plane. The idea behind such a contour is that it exploits the exponential factor in the Bromwich integral to produce a rapidly decaying integrand, which means that the integral can be approximated very efficiently by the trapezoidal rule.

In this talk we present a new idea in which we use (a) Gauss-Hermite quadrature on (b) a parabolic contour. On such a contour, the exponential factor in the Bromwich integral produces a Gaussian decay, which means that the integral can be approximated very efficiently by Hermite quadrature.

In both the Talbot method and the Hermite method there are a number of parameters that can be tuned for optimal accuracy. In the case of Talbot's method this has been done by the speaker and co-workers over the last decade or so. In this talk it is demonstrated how it can be done for the Hermite method, specifically for the important special case where the singularities of the transform occur on the negative real axis.

In several numerical experiments we show that, with an optimal choice of parameters for both methods, the Hermite method converges faster than the Talbot method. The improvement is not spectacular but in a typical problem the Hermite method might save two or three function evaluations. This can be significant when the transform is expensive to evaluate, such as when PDEs are solved.

Spectral approximation of convolution operator

Kuan Xu *(University of Kent)*

Convolution operator is ubiquitously dense in mathematics and engineering. While approximations for most commonly-seen operators, such as integration and differentiation, are well-known for decades and become indispensable in approximation theory and spectral methods for differential or integral equations, convolution operator hasn't been attempted much for approximations, particularly in coefficient space, until very recent years. In this talk, we will discuss the spectral approximation of convolution operator, based on orthogonal polynomials or Fourier series. The result enables accurate computation of convolution integrals using any family of orthogonal polynomial, such as Chebyshev, Legendre, and Gegenbauer, or Fourier series. We believe this work lays the foundation of the spectral methods for convolution integral equations.

A Shift-and-Invert Lanczos Algorithm for the Dynamic Analysis of Structures

Mante Zemaityte & Franoise Tisseur *(The University of Manchester)* & Ramaseshan Kannan *(Arup)*

Finding the response of a structure under dynamic loading is a crucial task in structure design. In particular, to accurately describe the behaviour of a building or a bridge when subjected to external forces, such as those induced by earthquakes or pedestrian footsteps, engineers require the smallest number of eigenvectors of the corresponding generalized eigenvalue problem that contribute by 90% to its total response.

Since not all eigenvectors contribute equally to describing the response of the structure, usually only a few eigenvectors are sufficient to achieve the 90% target. Those eigenvalues that correspond to the dominant eigenvectors tend to lie at the lower end of the spectrum, but since their exact location is not known in advance, one often computes an unnecessarily large number of eigenpairs, including those whose contribution to the total response is negligible.

By extending the theory on approximating the distribution of eigenvalues by the use of the Lanczos algorithm, we approximate the frequency intervals of eigenvalues corresponding to the dominant eigenvectors. We exploit this information by applying the shift-and-invert Lanczos algorithm to the problem and looking for eigenvalues only in those regions of the spectrum where eigenvalues corresponding to the dominant eigenvectors lie. This makes our approach faster and less memory intensive than existing methods.