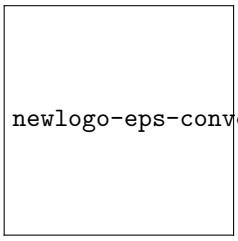


# 26th Biennial Conference on Numerical Analysis

23 – 26 June, 2015

## Contents

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## Introduction

Dear Participant,

On behalf of the Strathclyde Numerical Analysis and Scientific Computing Group, it is our pleasure to welcome you to the 26th Biennial Numerical Analysis conference. This is the fourth time the meeting has been held at Strathclyde, continuing the long series of conferences originally hosted in Dundee. This year we are particularly delighted to celebrate the $50^{th}$ anniversary of the very first meeting, which took place at the University of St Andrews in 1965, with four plenary speakers (D. Kershaw, J.D. Lambert, A.R. Mitchell and M.R. Osborne) and around 25 participants from the UK. The conference has since gone from strength to strength, with this year's meeting involving over 200 participants from 22 different countries across the world.

The conference is rather unusual in the sense that it seeks to encompass all areas of numerical analysis, and the list of invited speakers reflects this aim. We have once again been extremely fortunate in securing a top line-up of plenary speakers, and we very much hope that you enjoy sampling the wide range of interesting topics which their presentations will cover.

The meeting is funded almost entirely from the registration fees of the participants. Additional financial support for some overseas participants has come from the *Dundee Numerical Analysis Fund*, started by Professor Gene Golub from Stanford University in 2007. We are also indebted to the *City of Glasgow* for once again generously sponsoring a wine reception at the City Chambers on Tuesday evening, to which you are all invited.

We hope you will enjoy both the scientific and social aspects of the meeting, and look forward in particular to celebrating our Golden Anniversary in style at Wednesday evening's ceilidh dance and Thursday's Conference Dinner!

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**. Most meals will be served in the Aroma Dining Room in the Lord Todd building (building 26 on the campus map, entry as indicated). Breakfast is available from 07.30 until 09.00. The times of lunches and dinners are as indicated in the conference programme. A buffet lunch will be served on Friday 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, JA3.17, JA3.26 and JA3.27. 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 23rd June from 20.00 to 21.00. The City Chambers is marked on the campus map: entry is from George Square.
- **Ceilidh dance**. A celebration to mark 50 years since the first Biennial Numerical Analysis conference will be held on Wednesday 24th June at 18:30 (for 19:00 dinner) in the Barony Hall (building 30 on the campus map). This will take the form of a buffet meal, followed by some Scottish dancing.
- **Conference dinner**. The conference dinner will be held in the Auditorium of Òran Mór on Thursday 25th June at 19.30 (for 20:00 dinner). The venue is located at the top of Byres Road (G12 8QX): directions on how to travel there are provided in your conference folder. The guest speaker will be Professor Nick Higham, University of Manchester.
- **Internet Access**. Wireless access is available in all of the meeting rooms and in the Lord Todd bar/restaurant. 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 various facilities varies.

## Invited Speakers

| | | |
|---|---|---|
| Folkmar Bornemann | TU München | bornemann@tum.de |
| Susanne Brenner | Louisiana State University | brenner@math.lsu.edu |
| Albert Cohen | Université Pierre et Marie Curie | cohen@ann.jussieu.fr |
| Charlie Elliott | University of Warwick | c.m.elliott@warwick.ac.uk |
| Martin Gander | Université de Genève | Martin.Gander@unige.ch |
| Mike Giles | University of Oxford | Mike.Giles@maths.ox.ac.uk |
| Jan Hesthaven | EPFL | jan.hesthaven@epfl.ch |
| Tamara Kolda | Sandia National laboratories | tgkolda@sandia.gov |
| Cleve Moler | Mathworks | moler@mathworks.com |
| Michael Saunders | Stanford University | saunders@stanford.edu |
| Rob Scheichl | University of Bath | R.Scheichl@maths.bath.ac.uk |
| Karen Willcox | MIT | kwillcox@mit.edu |

# Abstracts of Invited Talks

### Random Matrix Distributions, Operator Determinants, and Numerical Noise

**Folkmar Bornemann** *(Technische Universität München, Germany)*

Because of universal scaling laws, distributions and correlation functions of classical random matrix ensembles and combinatorial growth processes in the large size limits have become increasingly important in physics and statistics. Their effective numerical computation has been made possible by evaluating higher derivatives of operator determinants. We review the underlying mathematical ideas and demonstrate how numerical explorations have led to new formulae, to new numerical algorithms, and finally allowed to exhibit universal scaling in some concrete physical experiments. Special attention is given to the sharp assessment of numerical errors: we relate them to a robust statistics of numerical noise in the tail of Chebyshev expansions.

### Finite Element Methods for Fourth Order Elliptic Variational Inequalities

**Susanne C. Brenner** *(Louisiana State University)*

Fourth order elliptic variational inequalities appear in obstacle problems for Kirchhoff plates and optimal control problems constrained by second order elliptic partial differential equations. The numerical analysis of these variational inequalities is more challenging than the analysis in the second order case because the complementarity forms of fourth order variational inequalities only exist in a weak sense. In this talk we will present a new approach to the analysis of finite element methods for fourth order elliptic variational inequalities that are applicable to C1 finite element methods, classical nonconforming finite element methods, and discontinuous Galerkin methods.

### Adaptive algorithms for high dimensional interpolation

**Albert Cohen** *(Université Pierre et Marie Curie, Paris)*

There exist many classical methods for interpolating a function of one or several variables. Practically all of these methods however face difficulties when considering functions of a large number of variables. We shall discuss and compare two approaches that can handle high dimensional data, the first based on Gaussian processes and the second based on sparse polynomial expansions. Both approaches give rise to adaptive greedy algorithms in which the interpolation points are chosen in a sequential manner, and which are still not well understood from a theoretical point of view. Our main motivation for this work is the non-intrusive treatment of parametric PDEs.

### Parabolic PDEs on evolving domains

**Charles Elliott** *(University of Warwick)*

I will discuss recent progress on the numerical analysis of PDEs on moving domains and in particular on the use of evolving finite element spaces.

### Linear and Non-Linear Preconditioning

**Martin J. Gander** *(Université de Genève)*

The idea of preconditioning iterative methods for the solution of linear systems goes back to Jacobi (1845), who used rotations to obtain a system with more diagonal dominance, before he applied what is now called Jacobi's method. The preconditioning of linear systems for their solution by Krylov methods has become a major field of research over the past decades, and there are two main approaches for constructing preconditioners: either one has very good intuition and can propose directly a preconditioner which leads to a favorable spectrum of the preconditioned system, or one uses the splitting matrix of an effective stationary iterative method like multigrid or domain decomposition as the preconditioner.

Much less is known about the preconditioning of nonlinear systems of equations. The standard iterative solver in that case is Newton's method (1671) or a variant thereof, but what would it mean to precondition the non-linear problem? An important contribution in this field is ASPIN (Additive Schwarz Preconditioned Inexact Newton) by Cai and Keyes (2002), where the authors use their intuition about domain decomposition methods to propose a transformation of the non-linear equations before solving them by an inexact Newton method. Using the relation between stationary iterative methods and preconditioning for linear systems, we show in this presentation how one can systematically obtain a non-linear preconditioner from classical fixed point iterations, and present as an example a new two level non-linear preconditioner called RASPEN (Restricted Additive Schwarz Preconditioned Exact Newton) with substantially improved convergence properties compared to ASPIN.

**Multilevel Monte Carlo methods**

**Mike Giles** *(University of Oxford)*

Monte Carlo methods are a standard approach for the estimation of the expected value of functions of random input parameters. However, to achieve improved accuracy one often requires more expensive sampling (such as a finer timestep discretisation of a stochastic differential equation) in addition to more samples. Multilevel Monte Carlo methods aim to avoid this by combining simulations with different levels of accuracy. In the best cases, the average cost of each sample is independent of the overall target accuracy, leading to very large computational savings.

The lecture will emphasise the simplicity of the approach, give an overview of the range of applications being worked on by various researchers, and also mention some recent extensions. Applications to be discussed will include financial modelling, engineering uncertainty quantification, stochastic chemical reactions, and the Feynman-Kac formula for high-dimensional parabolic PDEs.

Further information can be obtained from
`http://people.maths.ox.ac.uk/gilesm/acta/`

**High-order methods for fractional differential equations**

**Jan S Hesthaven** *(Ecole Polytechnique Fédérale de Lausanne)*

During the last few years, fractional calculus has emerged as an interesting tool to enable the modeling of a variety of problems often thought to be poorly modeled with classic calculus. Prominent examples suggesting a fractional model can be found in porous and granular flows, highly anisotropic problems, problems with inherent memory effects and can even emerge as a result of homogenization in multiscale problems.

While the idea of fractional calculus is as old as classic calculus, its theoretical and computational foundation is considerably less developed. Answers to seemingly simple questions of boundary conditions for fractional partial differential equations are often unknown. Furthermore, the nature of the fractional operators makes the development of computational techniques challenging because of the global and often singular nature of the solutions.

In this presentation we begin by providing some general background on fractional models and then discuss a few examples, including both fractional differential equations and fractional partial differential equations, of different high-order accurate computational methods, their analysis, and use. We shall conclude with a brief discussion of some of the many open problems.

**A Survey of Optimization Challenges in Tensor Decomposition**

**Tamara G Kolda**, *(Sandia National Laboratories)*

Tensors are multiway arrays, and tensor decomposition is a powerful tool for compression and data interpretation. In this talk, we survey the optimization approaches that have proved useful as well as open questions. We focus primarily on the canonical polyadic (CP) decomposition, also known as CANDECOMP or PARAFAC, which decomposes a tensor into a sum of rank-1 tensors. The standard approach to fitting a CP factorization is based on alternating least squares, but we also consider all-at-once optimization methods and discuss the special structure of the Hessian. For many real-world problems, the data is incomplete so we have to reformulate the optimization problem to account for the lack of data. A major open question is how to determine the number of components in the decomposition, and we present new results based on statistical cross-validation. We also consider special formulations of the CP problem, including symmetry constraints, coupled decompositions, alternate objective functions, and the best rank-one approximation (which finds a "tensor eigenpair"). We'll also briefly discuss optimization methods for the Tucker decomposition, which requires optimization on a manifold, and special methods for symmetric Tucker decompositions.

**Evolution of MATLAB**

**Cleve Moler** *(Mathworks)*

We show how MATLAB has evolved over more than 30 years from a simple matrix calculator to a powerful technical computing environment.We demonstrate several examples of MATLAB applications. We conclude with a discussion of current developments, including Parallel MATLAB for multicore and multicomputer systems.

Cleve Moler is the original author of MATLAB and one of the founders of the MathWorks. He is currently chairman and chief scientist of the company, as well as a member of the National Academy of Engineeringand past president of the Society for Industrial and Applied Mathematics.

See http://www.mathworks.com/company/aboutus/founders/clevemoler.html.

**Experiments with linear and nonlinear optimization using Quad precision**

**Michael Saunders** & Ding Ma *(Stanford University)*

For challenging numerical problems, William Kahan has said that "default evaluation in Quad is the humane option" for reducing the risk of embarrassment due to rounding errors. Fortunately the gfortran compiler now has a real(16) datatype. This is the humane option for producing Quad-precision software. It has enabled us to build a Quad version of MINOS.

The motivating influence has been increasingly large LP and NLP problems arising in systems biology. Flux balance analysis (FBA) models of metabolic networks generate multiscale problems involving some large data values in the constraints (stoichiometric coefficients of order 10,000) and some very small values in the solution (chemical fluxes of order $10^{-10}$). Standard solvers are not sufficiently accurate, and exact simplex solvers are extremely slow. Quad precision offers a reliable and practical compromise even via software. On a range of multiscale LP examples we find that 34-digit Quad floating-point achieves primal and dual infeasibilities of order $10^{-30}$ when "only" $10^{-15}$ is requested.

**Multilevel Uncertainty Quantification**

**Robert Scheichl** *(University of Bath)*

The term *Uncertainty Quantification* is as old as the disciplines of probability and statistics, but as a field of study it is newly emerging. It combines probability and statistics with mathematical and numerical analysis, large-scale scientific computing, experimental data, model development and application sciences to provide a computational framework for quantifying input and response uncertainties which ultimately can be used for more meaningful predictions with quantified and reduced uncertainty. We will motivate the central questions in computational uncertainty quantification through some illustrative examples from subsurface flow, weather and climate prediction and material science. The key challenge that we face in all those applications is the need for fast (tractable) computational tools for high-dimensional quadrature. Due to their tractability, Monte Carlo and other ensemble-type methods are the most widely used techniques, but especially when we want to combine input and output data in a Bayesian approach to inference they very quickly become too costly to be practically useful for large-scale scientific or engineering applications.

I will focus on multilevel (or multiscale) Monte Carlo methods that exploit the natural model hierarchies in numerical methods for differential equations to overcome this difficulty with a rigorous theoretical and practical control over bias and sampling errors. Most importantly it provides the genuine possibility to apply powerful, but typically expensive statistical tools, such as Metropolis-Hastings Monte Carlo Markov Chain (MCMC) or sequential Monte Carlo methods, in actual large-scale applications. In particular, I will present a multilevel MCMC algorithm with a computational cost that scales (at least in practice) optimally with respect to the required accuracy for a model problem in subsurface flow, as well as a complete numerical analysis of the method. I will finish my talk by pointing to some possible future research directions and potential applications for this promising new technology.

The work for this talk is based on collaborations with a large number of people, most notably my young colleagues Julia Charrier (Marseille), Tim Dodwell (Bath) and Aretha Teckentrup (Warwick).

**Data-Driven Model Reduction to Support Decision Under Uncertainty**

**Karen Willcox** *(Massachusetts Institute of Technology)*

Model reduction has become a powerful approach for extracting low-order, cheap surrogate models from high-fidelity simulation models, such as those arising from discretization of systems of partial differential equations. Recent developments in combining traditional projection-based model reduction methods with machine learning methods have led to new approaches that tune and adapt reduced models in the face of changing system properties and dynamic data. This provides new opportunities to discover and learn models, informed by physics-based first principles but guided by data. Our target is the next generation of complex engineered systems, which will be endowed with sensors and computing capabilities that enable new modes of decision-making. For example, new sensing capabilities on aircraft will be exploited to assimilate data on system state, make inferences about system health, and issue predictions on future vehicle behavior—with quantified uncertainties—to support critical operational decisions. Model reduction is one way to achieve this challenging task, in particular through data-driven reduced models that exploit the synergies of physics-based computational modeling and physical data.

This talk will provide a brief overview of the basics of model reduction and discuss some of our recent work in data-driven reduced model localization and adaptation. I will also offer some future directions in multi-

information-source approaches that aim to create a principled strategy for managing high-fidelity models, reduced models, and data in a design setting.

# Minisymposia abstracts

Minisymposium M1

Stable and accurate discretisations for convection-dominated problems
Organisers
Gabriel Barrenechea and Natalia Kopteva

### Adaptive time step control with variational time stepping schemes for convection-diffusion-reaction equations

**Naveed Ahmed** & Volker John *(Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Germany,)*

Higher order variational time stepping schemes allow an efficient post-processing for computing a higher order solution. In this talk, we present an adaptive algorithm whose time step control utilizes the post processed solution. As a model problem, we will consider the convection-dominated convection-diffusion-reaction equations. In particular, for the space discretization of convection-diffusion-reaction equations, we will consider the streamline upwind-Petrov Galerkin method as stabilization. Moreover, the continuous Galerkin-Petrov (cGP) and discontinuous Galerkin (dG) schemes will be used as time discretization.

At first step, for fixed time step and for smooth solution, we will show that the cGP($k$) and dG($k$) with $k$ the polynomial degree with respect to time are of order $k+1$ in the integrated $L^2(L^2)$ time-space norm and the post processed solution is of order $k+2$ in the corresponding norm. Furthermore, at discrete time points, we obtain a super-convergence of order $2k$ and $2k+1$ for cGP($k$) and dG($k$) methods, respectively.

The availability of two solutions with different order enables also the application of well understood techniques from the numerical analysis of ordinary differential equations for controlling the adaptive time step. We will apply the adaptive algorithm based on the PID and PC11 controllers. The performance of the cGP and dG methods will be compared with the performance of (a slight modification of) the adaptive Crank-Nicolson scheme proposed, which is based on controlling the time step with the solution obtained with the Adams-Bashforth scheme. Several numerical tests have been made to show the performance of different time stepping schemes.

### A robust numerical method for a control problem of singularly perturbed equations

**Alejandro Allendes** & Erwin Hernández & Enrique Otarola *(University Técnica Federico Santa María, Chile, University of Maryland and George Mason University, USA)*

We consider a linear–quadratic optimal control problem governed by a singularly perturbed convection–reaction–diffusion equation. Since we do not consider constraints on the control, the optimality system associated with the optimal control problem consists of a coupled system involving both the state and adjoint equations. We analyze and discretize the optimality system by using standard bilinear finite elements on the graded meshes introduced by Durán and Lombardi [1,2 ]. We derive quasi-optimal a priori error estimates for the optimal variables on anisotropic meshes. Finally, we present several numerical experiments which reveal a competitive performance of our method compared with adaptive stabilized schemes.

#### References

[1] R.G. Durán and A.L. Lombardi, *Error estimates on anisotropic $Q_1$ elements for functions in weighted Sobolev spaces*. Math. Comp., 74(252):1679–1706 (electronic), 2005.
[2] R.G. Durán and A.L. Lombardi, *Finite element approximation of convection diffusion problems using graded meshes*. Appl. Numer. Math., 56(10-11): 13141325, 2006.

### Stability and error analysis of algebraic flux correction schemes

**Gabriel R. Barrenechea** & Volker John & Petr Knobloch *(University of Strathclyde, Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Germany, Charles University in Prague)*

A family of algebraic flux correction schemes for linear boundary value problems in any space dimension is studied. These methods' main feature is that they limit the fluxes along each one of the edges of the triangulation, and we suppose that the limiters used are symmetric. For an abstract problem, the existence of a solution, existence and uniqueness of the solution of a linearized problem, and an a priori error estimate, are proved under rather general assumptions on the limiters. For a particular (but standard in practice) choice of the limiters, it is shown that a local discrete maximum principle holds. The theory developed for the abstract problem is applied to convection–diffusion–reaction equations, where in particular an error estimate is derived. Numerical studies

show its sharpness.

### *hp*–Version discontinuous Galerkin methods on polytopic meshes

**Andrea Cangiani**, Zhaonan Dong, Emmanuil Georgoulis *(University of Leicester)* & Paul Houston *(University of Nottingham)*

We present recent work on *hp*–version interior penalty discontinuous Galerkin finite element methods (DGFEM) for advection–diffusion–reaction equations on general computational meshes consisting of polygonal/polyhedral (polytopic) elements [2, 1]. The proposed methods employ elemental polynomial bases of total degree $p$ ($\mathcal{P}_p$–basis) defined in the physical coordinate system, without requiring the mapping from a given reference or canonical frame. New *hp*–version *a priori* error bounds are derived based on a specific choice of the interior penalty parameter which allows for edge/face–degeneration. Numerical experiments highlighting the performance of the proposed DGFEM are presented.

#### References

[1] A. Cangiani, Z. Dong, E.H. Georgoulis, and P. Houston. *hp*–version discontinuous galerkin methods for advection–diffusion–reaction problems on polytopic meshes. Submitted.
[2] A. Cangiani, E.H. Georgoulis, and P. Houston. *hp*–version discontinuous Galerkin methods on polygonal and polyhedral meshes. *Math. Models Methods Appl. Sci.*, 24(10):2009–2041, 2014.

### Monotonicity Preserving Techniques for Continuous and Discontinuous Galerkin Methods

**Alba Hierro** & Santiago Badia *(UPC,CIMNE)*

It is well known that spurious oscillations may appear when using finite elements for solving problems that present shocks or sharp layers. In particular this might happen when solving the time-dependent transport equation or convection dominant convection-diffusion problems. There are several ways to avoid this behaviour, in particular it is quite common to add artificial diffusion in the area where the shocks are detected.

A particular desirable feature for the methods is to enjoy the discrete maximum principle (DMP). The DMP ensures that the discrete solution inherits the monotonicity of the continuous problem. The authors propose a monotonicity preserving shock detector that might be used for continuous and discontinuous Galerkin methods.

Moreover, for the continuous case, the nonlinear artificial diffusion is usually combined with a linear stabilization term in order to improve the results. The authors have proposed a symmetric nodal projection stabilization together with a blending factor that keeps the monotonicity of the method. On the other hand, also the Interior Penalty discontinuous Galerkin terms have been arranged in order for the method to be monotonic in 1D.

Currently the authors are working on the implementation of such features on *hp*-adaptive meshes. In particular, it is necessary to properly detect the shock regions to be able to impose linear order to the elements.

### Local projection type stabilisation applied to inf-sup stable discretisations of the Oseen problem

**Gunar Matthies** & Lutz Tobiska *(Technische Universität Dresden)*

We consider the Oseen problem

$$-\nu\triangle u + (b\cdot\nabla)u + \sigma u + \nabla p = f \text{ in } \Omega,$$
$$\text{div } u = 0 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega,$$

where $\nu > 0$ and $\sigma \geq 0$ are constants and $b \in \left(W^{1,\infty}(\Omega)\right)^d$ with div $b = 0$ is a given velocity field. The Oseen problem can be considered as a linearisation of the steady ($\sigma = 0$) and the time-discretised non-steady ($0 < \sigma \sim 1/\triangle t$) Navier–Stokes equations, respectively.

Inf-sup stable finite element discretisations of the Oseen problem are considered. Hence, no additional pressure stabilisation is needed. However, the standard Galerkin method still suffers in general from global spurious oscillations in the velocity field which are caused by the dominating convection.

Local projection stabilisation methods will be used to overcome this difficulty. The stabilisation is based on a projection from the underlying approximation space onto a discontinuous projection space. Stabilisation is derived from additional weighted $L^2$-control on the fluctuation of the gradient of the velocity or only parts of it like divergence and/or derivative in streamline direction.

The convergence analysis for both the one-level and the two-level local projection stabilisation applied to inf-sup stable discretisations of the Oseen problem will be presented in a unified framework.

Two different stabilisation terms are considered. The

first stabilisation introduces control over the fluctuations of the derivative in streamline direction and over the fluctuations of the divergence separately whereas the second stabilisation controls the fluctuations of the gradient.

We will propose new inf-sup stable pairs of finite element spaces which approximate both velocity and pressure by elements of order $r$. In contrast to the classical equal order interpolation, the velocity components and the pressure are discretised by different elements. We will show the discrete inf-sup condition for these pairs of finite element spaces. For the case of small viscosity, a uniform error estimate of order $r + 1/2$ will be proved. In the case of discontinuous pressure approximations, an additional term controlling the jumps of the pressure across inner cell faces becomes necessary.

Numerical tests which confirm the theoretical results will be given.

### Local error estimates for the SUPG method applied to evolutionary convection-reaction-diffusion equations

Javier de Frutos, Bosco García-Archilla & **Julia Novo** *(University of Seville)*

Local error estimates for the SUPG method applied to evolutionary convection-reaction-diffusion equations are considered. The steady case is reviewed and local error bounds are obtained for general order finite element methods. For the evolutionary problem, local bounds are obtained when the SUPG method is combined with the backward Euler scheme. The arguments used in the proof lead to estimates for the stabilization parameter that depend on the length on the time step. The numerical experiments show that local bounds seem to hold true both with a stabilization parameter depending only on the spatial mesh grid and with other time integrators.

### Multiscale Hybrid-Mixed Method for Advective-Reactive Dominated Problems with Heterogeneous Coefficients

Rodolfo Araya & Christopher Harder & **Diego Paredes** & Frédérid Valentin *( Universidad de Concepción, Chile, Metropolitan State University of Denver, Pontifical Catholic University of Valparaíso - IMA/PUCV, Laboratório Nacional de Computação Científica - LNCC, Brazil)*

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

**Keywords**: reaction-advection-diffusion, multiscale, mixed-hybrid, adaptivity
**Mathematics Subject Classifications (2000)**:

#### References

[1] C. Harder and D. Paredes and F. Valentin A Family of Multiscale Hybrid-Mixed Finite Element Methods for the Darcy Equation with Rough Coefficients. In: *Journal of Computational Physics* Vol. 245, pp. 107-130, 2013.
[2] R. Araya and C. Harder and D. Paredes and F. Valentin Multiscale Hybrid-Mixed Methods. In: *SIAM Journal on Numerical Analysis* Vol. 51(6), pp. 3505-3531, 2013.
[3] C. Harder and D. Paredes and F. Valentin On a Multiscale Hybrid-Mixed Method for Advective-Reactive Dominated Problems with Heterogenous Coefficients. In: *Multiscale Modeling & Simulation* Vol. 13(2), pp. 491-518, 2015.

### Virtual Element Methods for Elliptic Problems

**Oliver Sutton** & Andrea Cangiani *(University of Leicester)* & Gianmarco Manzini *(LANL)*

The virtual element method is a recent generalisation of the standard conforming finite element method to meshes consisting of arbitrary (convex or non-convex) polygonal elements, and may be viewed as the variational analogue of the mimetic finite difference method. Despite being only recently introduced, the virtual element method has already been applied to a wide variety of different problems, including the Poisson

problem, plate-bending and linear elasticity problems, Stokes problem, the Steklov eigenvalue problem and the simulation of discrete fracture networks. However, until recently an exposition of the method for linear elliptic problems with non-constant coefficients has been lacking. In this talk, we will discuss ongoing work to extend the virtual element methodology to this class of problems and the modifications to the original virtual element framework which were necessary to produce a practical method.

## Minisymposium M2

## Kernel Methods in Numerical Analysis and Learning Theory

Organisers

Jeremy Levesley and Holger Wendland

### Learning functions on data defined manifolds

**Frank Filbir** *(Helmholtz Zentrum München)*

Many practical applications, for example, document analysis, face recognition, semi-supervised learning, and image processing, involve a large amount of very high dimensional data. Typically, this data has a lower intrinsic dimensionality; for example, one may assume that it belongs to a low dimensional manifold in a high dimensional, ambient Euclidean space. The desire to take advantage of this low intrinsic dimensionality has recently prompted a great deal of research on diffusion geometry techniques. In this talk we will demonstrate how kernel techniques can be linked with this approach in order to learn functions on such data defined manifolds.

### Scaling inference for Gaussian processes using stochastic linear algebra techniques

**Maurizio Filippone** *(University of Glasgow)*

Probabilistic kernel machines based on Gaussian Processes (GPs) are popular in several applied domains due to their flexible modelling capabilities and interpretability. In applications where quantification of uncertainty is of primary interest, it is necessary to carry out Bayesian inference of GP covariance parameters (kernel parameters), and this would require repeatedly calculating the marginal likelihood of GP models. The formidable computational challenge associated with this is that the marginal likelihood is only computable in the case of GP models applied to regression problems. Even then, for large datasets, it is not possible to compute the marginal likelihood exactly. This is because computing the marginal likelihood entails storing and factorising the kernel matrix, which is generally dense, requiring $O(n^2)$ storage and $O(n^3)$ computations, $n$ being the number of input data. This has motivated the research community to develop a variety of approximation techniques. Even though such approximations make it possible to recover computational tractability, it is not possible to determine to what extent they affect the performance of GP-based models.

A recent trend in the area of scalable Bayesian inference is developing inference techniques based on "mini-batches", namely methods that combine computations carried out on subsets of the data without introducing any bias in the inference process. The Stochastic Gradient Langevin Dynamics (SGLD) algorithm [Welling and Teh, ICML, 2011], for example, uses mini-batches to estimate the gradient of the log-likelihood unbiasedly. The appeal of SGLD is that, at the expense of introducing an asymptotically vanishing amount of bias, inference can be carried out without having to compute the likelihood and without the need to compute the gradient of the log-likelihood exactly, resulting in tremendous computational savings.

The applicability of SGLD and many other inference methods based on mini-batches hinges on the factorisation properties of the likelihood. When this is not the case, these methods cannot be directly applied. GP-based statistical models offer a perfect example of a class of models where the marginal likelihood does not factorise, but reducing computational complexity is highly desirable due to the poor scalability of traditional likelihood-based inference methods.

This work proposes Bayesian inference for GP regression using an adaptation of SGLD where an unbiased estimate of the gradient of the log-marginal likelihood is calculated employing stochastic linear algebra techniques, leading to an expression involving dense linear systems only. This has the enormous advantage that dense linear systems can be solved iterating matrix-vector products that (i) are highly parallelisable, (ii) do not require storing the kernel matrix leading to $O(n)$ storage, and (iii) require $O(n^2)$ computations. Furthermore, a novel unbiased linear systems solver is developed to accelerate the unbiased estimation of the gradient of the log-marginal likelihood needed by SGLD. The results demonstrate the possibility to enable scalable and exact (in a Monte Carlo sense) Bayesian inference for Gaussian processes.

### A High-Order, Analytically Divergence-free Approximation Method for the Navier-Stokes Equations

**Christopher Keim** *(University of Bayreuth)*

We present a new high-order approximation method for the incompressible Navier-Stokes equations using collocation in space and a method of line approach to split variables. Our spatial approximation space consists of smooth, analytically divergence-free functions based on specifically designed matrix-valued kernels. Besides yielding analytically divergence-free approximations of the velocity, our approximation scheme has the additional advantages that no mesh has to be generated, no numerical integration is required and that the velocity and pressure part of the approximate solution are computed simultaneously. No inf-sup condition nor the solution of an additional Poisson problem is required.

For simplicity, our analysis will be restricted to the case of periodic boundary conditions. We will give exact error bounds for the semi-discrete scheme and also for the fully discretised system.

**Filtering and parameter estimation of partially observed diffusion processes using Gaussian RBFs**

**Elisabeth Larsson**, Josef Höök, Erik Lindström, & Lina von Sydow *(Uppsala University)*

Financial asset prices can be modeled as stochastic diffusion processes involving a number of parameters. Based on market observations over time, we want to estimate these parameters. However, due to the so called ask-bid spread, there is an uncertainty in the observed data. We model the spread as additive noise, and show that using Gaussian radial basis functions (RBFs), leads to a convenient mathematical representation. Furthermore, substantial parts of the computations can be performed analytically if RBFs are used for approximating transition densities. We present numerical results for a short term interest rate model showing that we can generate a smooth likelihood surface.

**Grid Refinement in the Construction of Lyapunov Functions Using Radial Basis Functions**

**Najila Mohammed** *(Sussex University)*

Meshless collocation based on Radial basis functions, kernel functions, is an effective tool to solve Linear PDE's. Moreover, **RBFs** can be used to construct Lyapunov functions, such that their existence guarantees determining subsets of the domain of attraction of an equilibrium of an ODE.

In this talk, a new grid refinement strategy associated with this construction method will be presented and illustrated in examples.

**Approximation of Lyapunov Functions from Data**

**Kevin Webster,** Peter Giesl, Boumediene Hamzi & Martin Rasmussen *(Imperial College London)*

Methods have previously been developed for the approximation of Lyapunov functions using radial basis functions. However these methods assume that the evolution equations are known. We consider the problem of approximating a given Lyapunov function using radial basis functions where the evolution equations are not known, but we instead have sampled data which is contaminated with noise. Our approach is to first approximate the underlying vector field, and use this approximation to then approximate the Lyapunov function. Our approach combines elements of machine learning/statistical learning theory with the existing theory of Lyapunov function approximation. Error estimates are provided for our algorithm.

**A high-order, analytically divergence-free approximation method for the time-dependent Stokes problem**

**Holger Wendland** & Christopher Keim *(University of Bayreuth)*

In this talk, I will present and analyse a new high-order approximation method for the time-dependent Stokes equation. The new method is based upon an analytically divergence-free approximation space using smooth, matrix-valued kernels. This method has several advantages. It is a truly meshfree method. It allows us to reconstruct the velocity and the pressure part of the solution simultaneously, without solving an additional Poisson problem and without the requirement of an inf-sup condition. Moreover, since we use collocation in space no numerical integration is required. I will give explicit error bounds for the semi-discrete approximation as well as for the fully discretised system.

**Radial Basis Functions Interpolation with Error Indicator**

**Qi Zhang** & Jeremy Levesley *(University of Leicester)*

Radial Basis Functions (RBF) methods have been gaining attention by their simplicity and ease of implementation in multivariate scattered data approximation. My study focuses on applying RBF interpolation to build a surrogate model for an unknown target func-

tion $f$ within limited resources while providing a sufficient accuracy level.

In order to achieve satisfying accuracy levels of the model, the resources should be carefully selected and used. In this case, the resources are the scattered nodes measured form the target function. Compared to using all the scattered nodes in one time to build a whole domain interpolant, domain decomposition methods give out better accuracy and also less conditioning problems.

In my model, a domain decomposition method is applied. Firstly, a whole domain interpolant $S$ based on well distributed nodes is established which approximates the target function. Secondly, Error Indicator is involved to detect the error of $S$, it should be able to detect the sub-domains where the error is large. Thirdly, local error correction interpolants are used to correct the error at previously decided sub-domains. By repeating the second and third steps, the model could reach its pre-set accuracy level.

Error Indicators use polyharmonic spline basis functions to reconstruct a local approximation $S_{local}$ without using extra nodes. The deviation between $S_{local}$ and $f$ indicates the error level in this sub-domain. By continuously applying the Error Indicator, an adaptive nodes distribution is gained.

**Analogues of Classical Results on Radial Basis Functions for Zonal Basis Functions on the Sphere**

**Wolfgang zu Castell** & Rick Beatson, Yuan Xu *(Helmholtz Zentrum München)*

Several properties of basis functions used for interpolation and approximation in Euclidean spaces can be derived from Bochner's Theorem characterising radial positive definite functions. The same type of equivalence has been stated by Schoenberg for zonal basis functions on the sphere.

The spherical functions characterising this geometric set-up are given by Gegenbauer polynomials. Aiming at transferring well-established results from radial basis function approximation to the geometric setting of the sphere, certain properties of Gegenbauer polynomials are needed. While some of these properties are already known, others lead to interesting problems dealing with this family of orthogonal polynomials.

## Minisymposium M3

## Recent developments of mathematical aspects of computational chemistry

Organiser
Benjamin Stamm

**Computational methods for the dynamics of the Gross-Pitaevskii/nonlinear Schrödinger equation with rotation and dipole-dipole interaction**

**Weizhu Bao** *(National University of Singapore)*

In this talk, I begin with the Gross-Pitaevskii/ nonlinear Schrödinger equation (GPE/NLSE) with an angular momentum rotation and/or a dipole-dipole interaction for modeling rotating and/or dipolar Bose-Einstein condensation (BEC), and review some dynamical properties of GPE/NLSE including conserved quantities and center-of-mass dynamics. Different numerical methods will be presented and compared. Applications to simulate the dynamics of rotating BEC and/or dipolar BEC will be reported. Finally, extension to coupled GPEs with a spin-orbit coupling will be discussed.

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**Greedy algorithms for electronic structure calculations for molecules**

Eric Cancès & **Virginie Ehrlacher** & Majdi Hochlaf & Tony Lelièvre *(CERMICS, Ecole des Ponts Paristech & INRIA)*

In this talk, a greedy algorithm will be presented in order to compute the lowest eigenvalue and an associated eigenstate for high-dimensional problems and their numerical behaviour will be illustrated for the computation of the ground-state electronic wavefunction of a molecule, solution of the many-body Schrödinger equation. Usually, these algorithms are implemented in practice using the Alternating Least-Square algorithm, which leads to some computational difficulties in this particular situation due to the anti-symmetry of the ground state wavefunction. A computational strategy to overcome this difficulty will be presented and illustrated on several molecules.

**Large-scale real-space electronic structure calculations**

**Vikram Gavini** & Phani Motamarri *(University of Michigan, Ann Arbor)*

In this talk, the development of a real-space formulation for Kohn-Sham density functional theory (DFT) and a finite-element discretization of this formulation [1], which can handle arbitrary boundary conditions and is amenable to adaptive coarse-graining, will be presented. In particular, the accuracy afforded by using higher-order finite-element discretizations, and the efficiency and scalability of the Chebyshev filtering algorithm in pseudopotential and all-electron Kohn-Sham DFT calculations will be demonstrated. Further, the development of a subquadratic-scaling approach (in the number of electrons) based on a subspace projection and Fermi-operator expansion will be discussed [2], which will be the basis for the future development of coarse-graining techniques for Kohn-Sham DFT. The developed techniques have enabled, to date, pseudopotential calculations on non-periodic and periodic systems containing $\sim$ 10,000 atoms, as well as all-electron calculations on systems containing $\sim$ 5,000 electrons.

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**A posteriori error estimates for Discontinuous Galerkin methods using non-polynomial basis functions with applications to solving Kohn-Sham density functional theory**

**Lin Lin** & Benjamin Stamm *(University of California, Berkeley and Lawrence Berkeley National Laboratory)*

Recently we have developed the adaptive local basis functions in a discontinuous Galerkin framework for reducing the dimension of the discretized system for solving the Kohn-Sham density functional theory. The discontinuous Galerkin method provides a natural framework for reducing the dimension of the system obtained by discretizing a PDE, due to its ability to incorporate an efficient non-polynomial basis set, without the need to match the value of such basis functions at the boundary. However, the use of non-polynomial basis functions lead to major difficulties in error analysis, both in the a priori and the a posteriori sense. We present, to the extent of our knowledge, the first systematic work for deriving a posteriori error estimates for general non-polynomial basis functions in an interior penalty discontinuous Galerkin (DG) formulation for solving second order linear PDEs. Our residual type upper and lower bound error estimates measures the error in the energy norm. The main merit of our method is that the method is parameter-free, in the sense that all but one solution-dependent constant appearing in the upper and lower bound estimates are explicitly computable, and the only non-computable constant can be reasonably approximated by a computable one without affecting the overall effectiveness of the estimates in practice. We develop an efficient numerical procedure to compute the error estimators. Numerical results for a variety of problems in 1D and 2D demonstrate that both the upper bound and lower bound are effective. We demonstrate some practical use of a posteriori error estimators in performing three-dimensional Kohn-Sham density functional theory calculations for quasi-2D aluminum surfaces and single-layer graphene oxide in water.

**Fast domain decomposition methods for continuum solvation models**

**Filippo Lipparini** & Benjamin Stamm, & Eric Cancès & Yvon Maday & Benedetta Mennucci *(Johannes Gutenberg Universität, Mainz)*

Continuum solvation models are very popular tools in computational chemistry. In the last three decades, they have allowed computational chemists to reproduce environmental effects on molecular structures and properties in quantum-mechanical (QM) simulations performed with various levels of theory in a cost-effective, but fairly accurate, way. However, such models were originally formulated thinking of a pure QM description of the solute: due to the high computational cost associated with solving the QM equations, the systems treated have always been medium-sized or small, which made the cost of solving the linear equations associated to the continuum solvation mod-

els negligible with respect to the effort required by the overall computation. Recently, thanks to the increase in computer power, to the development of state-of-the-art linear scaling algorithms and, most important, to the development of hybrid quantum-classical methods, large and very large molecular systems have become accessible: for systems as large as a protein (beyond one thousand atoms), the continuum solvation equations with existing implementations can become prohibitive.

In this contribution, we present a new discretization for COSMO (Conductor-like screening model), a very popular continuum solvation model, based on a domain-decomposition approach. We refer to our new algorithm as ddCOSMO. After summarizing some mathematical aspects of the procedure, we will describe the algorithm and focus on the numerical details. We will show, including some examples, that our implementation scales linearly in computational cost and memory requirements with respect to the size of the solute and allows us to treat large and very large systems with a cost which is a small fraction of the cost of the simulation *in vacuo*. Compared to the most efficient existing implementations, ddCOSMO is two to three orders of magnitude faster, more robust and defined by a smaller number of discretization parameters: these features allow us to extend the applicability of continuum solvation models to large and complex biological and chemical systems in combination with classical, QM and hybrid descriptions of the solute.

### Quantum Calculations in Solution for Large to Very Large Molecules: presentation of the mathematical algorithm

**Yvon Maday** & Filippo Lipparini, Louis Lagardère, Giovanni Scalmani, Benjamin Stamm, Eric Cancès , Jean-Philip Piquemal, Michael J. Frisch and Benedetta Mennucci *(Sorbonne Universités, UPMC Univ Paris 06, Univ. Paris Diderot, Sorbonne Paris Cité, CNRS, Institut Universitaire de France, Laboratoire Jacques-Louis Lions, France and Division of Applied Mathematics, Brown University )*

We present a new algorithm of continuum solvation models for semiempirical Hamiltonians that allows the description of environmental effects on large to very large molecular systems. In this approach based on a domain decomposition strategy of the COSMO model (ddCOSMO), the solution to the COSMO equations is no longer the computational bottleneck but becomes a negligible part of the overall computation time. In this presentation, we present the algorithm in light of existing works in the field of domain decomposition for elliptic problems, we analyze the computational impact of COSMO on the solution of the SCF equations for large to very large molecules, using semiempirical Hamiltonians, for both the new ddCOSMO implementation and the most recent, linear scaling one, based on the fast multipole method. The approach is illustrated with a few examples that will be extended to larger problems of interest in the chemical community in the talk of F. Lipparini.

### A perturbation-method-based post-processing of planewave approximations for nonlinear Schrödinger equations

**Benjamin Stamm** & Eric Cancès, Geneviève Dusson, Yvon Maday, Martin Vohralìk *(Sorbonne Université UPMC Paris 6 and CNRS)*

In this talk we consider a post-processing of planewave approximations for nonlinear Schrödinger equations by considering the exact solution as a perturbation of the discrete, computable solution. Applying then Katos perturbation theory leads to computable corrections with a provable increase of the convergence rate in the asymptotic range for a very little computational overhead. We illustrate the key-features of this post-processing for the Gross-Pitaevskii equation that serves as a toy problem for DFT Kohn-Sham models. Finally some numerical illustrations in the context of DFT Kohn-Sham models are presented.

### Absorption Spectrum Estimation via Linear Response Time-dependent Density Functional Theory

**Chao Yang** & Jiri Brabec & Lin Lin *(Lawrence Berkeley National Laboratory)* & Yousef Saad *(University of Minnesota)*

The absorption spectrum of a molecular system can be estimated from the dynamic dipole polarizability associated with the linear response of a molecular system (at its ground state) subject to an external perturbation. Although an accurate description of the absorption spectrum requires the diagonalization of the so-called Casida Hamiltonian, there are more efficient ways to obtain a good approximation to the general profile of the absorption spectrum without computing eigenvalues and eigenvectors. We describe these methods which only require multiplying the Casida Hamiltonian with a number of vectors. When highly accurate oscillator strength is required for a few selected excitation energies, we can use a special iterative method to obtain the eigenvalues and eigenvectors associated with these energies efficiently.

Minisymposium M4

Numerical Methods in Stochastic Problems in Biology
Organisers
S. Cotter and K. Zygalakis

**A constrained approach to the simulation of multiscale chemical kinetics**

**Simon Cotter** *(University of Manchester)*

In many applications in cell biology, the inherent underlying stochasticity and discrete nature of individual reactions can play a very important part in the dynamics. The Gillespie algorithm has been around since the 1970s, which allows us to simulate trajectories from these systems, by simulating in turn each reaction, giving us a Markov jump process. However, in multiscale systems, where there are some reactions which are occurring many times on a timescale for which others are unlikely to happen at all, this approach can be computationally intractable. Several approaches exist for the efficient approximation of the dynamics of the "slow" reactions, many of which rely on the "quasi-steady state assumption". In this talk, we will present the Constrained Multiscale Algorithm, a method which was previously used to construct diffusion approximations of the slowly changing quantities in the system, but which does not rely on the QSSA. We will show how this method can be used to approximate an effective generator for the slow variables in the system, and quantify the errors in that approximation. If time permits, we will show how these generators can then be used to sample approximate paths conditioned on the values of their endpoints.

**A comparison of approximation methods for stochastic biochemical networks**

**Ramon Grima** *(University of Edinburgh)*

Exact solutions of the chemical master equation are only known for a handful of simple chemical systems and stochastic simulations are typically computationally expensive. In the past decade, the linear-noise approximation (LNA), the chemical Fokker-Planck equation (CFPE) and moment-closure approximations (MA) have become a popular means to efficiently approximate the master equation and to hence obtain insight into the effect of noise on the dynamics of biochemical systems. However these approximations are plagued by a number of problems in particular their accuracy and their relationship to one another remains unclear furthermore, the most popular of these methods, the LNA, can only be applied to a subset of reaction systems, namely those characterised by a unimodal probability distribution and provided the molecule numbers are quite large. In this talk, I will present an overview of our work over the past few years which clarifies the accuracy of the LNA, CFPE and MA approximations. I will also present modifications to the LNA which enables its application to multimodal systems and those in which one more more species are present in few molecule numbers. The usefulness of these methods to obtaining a more complete picture of stochastic biochemical dynamics will be showcased on various biochemical systems involving gene expression, feedback control, enzyme-mediated catalysis and circadian rhythms.

**Hybrid modelling of stochastic chemical kinetics**

**Kostas Zygalakis** *(University of Southampton)*

It is well known that stochasticity can play a fundamental role in various biochemical processes, such as cell regulatory networks and enzyme cascades. Isothermal, well-mixed systems can be adequately modelled by Markov processes and, for such systems, methods such as Gillespie's algorithm are typically employed. While such schemes are easy to implement and are exact, the computational cost of simulating such systems can become prohibitive as the frequency of the reaction events increases. This has motivated numerous coarse grained schemes, where the "fast" reactions are approximated either using Langevin dynamics or deterministically. While such approaches provide a good approximation for systems where all reactants are present in large concentrations, the approximation breaks down when the fast chemical species exist in small concentrations, giving rise to significant errors in the simulation. This is particularly problematic when using such methods to compute statistics of extinction times for chemical species, as well as computing observables of cell cycle models. In this talk, we present a hybrid scheme for simulating well-mixed stochastic kinetics, using Gillepsie–type dynamics to simulate the network in regions of low reactant concentration, and chemical Langevin dynamics when the concentrations of all species is large. These two regimes are coupled via an intermediate region in which a "blended" jump-diffusion model is introduced. Examples of gene regulatory networks involving reactions occurring at multiple scales, as well as a cell-cycle model are simulated, using the exact and hybrid scheme, and compared, both in terms of weak error, as well as computational cost.

Minisymposium M5

City Analytics
Organisers
Des Higham and Jeremy Levesley

**Communicability Angles and the Spatial Efficiency of City Networks**

**Ernesto Estrada** & Naomichi Hatano *(University of Strathclyde, University of Tokyo, Japan)*

We introduce the concept of communicability angles between a pair of nodes in a graph. We provide strong analytical and empirical evidence that the average communicability angle for a given network accounts for its spatial efficiency on the basis of the effectivity of communication among the nodes in a network. We determine the spatial efficiency characteristics of more than 100 real-world complex networks representing complex systems arising in a diverse set of scenarios. In particular, we illustrate our results with the study of a few urban street networks for different cities around the world. We finally show how the spatial efficiency of a network can be modulated by tuning the weights of the edges of the networks. This allows us to predict the effects of external stress over the spatial efficiency of a network as well as to design strategies to improve that important parameter in real-world complex systems.

**Numerical Analyticity**

**Desmond J. Higham**, *University of Strathclyde*

We may view the city as a *living lab*, where human activity is now generating vast arrays of data. For example, we can make observations around online social media, telecommunication, geolocation, crime, health, transport, air quality, energy, utilities, weather, CCTV, wi-fi usage, retail footfall and satellite imaging. These emerging data sets, and accompanying research questions, have the potential to motivate new and useful mathematics. I will give a personal overview of some of the key challenges for applied and computational mathematicians. In particular, I will discuss activity taking place in Glasgow, which was chosen as the UK's Smart Demonstrator City, and in the University of Strathclyde's Institute for Future Cities.

**Urban Living: Towards a Comparison of City-based Digital Social Networks and of Individual Demand Behaviour (Part 1 and Part 2)**

**Peter Grindrod** & **Tamsin Lee** *(University of Oxford)*

Urban living will unceasingly be examined under the digital microscope of Future City programmes. As digital communication platforms become more ubiquitous and the digital monitoring and demand behaviour for consumers and lifestyle products and services becomes more prevalent, we shall be able to move away from a "one shoe fits all" approach to anticipating and fulfilling citizens' demands, needs, and aspirations. A crucial step is to allow human behaviour, and behavioural data, of individuals, communities, boroughs and whole cities to speak for itself. Here we shall consider what analytics is available in order to extract insights from two distinct types of behavioural data: peer-to-peer (P2P) communication within online social media, indicating hidden social structures; and business-to-customer (B2C) interactions, here regarding domestic and light commercial energy demand behaviour. In the first case we shall consider ten large British cities as they are represented by social networks: our analysis of these networks deploys a range of approaches, and indicates that these P2P communities are not necessarily the same—urban societies within cities may fall into classes, and this should evolve in time. In the latter case it is individuals behaviour (private consumption) that is diverse and our analysis suggests that behavioural segmentations are necessary to anticipate and manage smallish aggregates (100 home or less) on local distribution networks. Looking to the future we must develop operational algorithms to forecast and manage behaviour that can scale up in size (up to full penetration of our largest cities) and scale efficiencies to make 24/7 management and response a reality—including within emergency scenarios, such as power outages where energy distribution and intelligence sourced form social media intersect. We shall focus on the wide range mathematical methods underpinning such analytics.

**Sparse interpolation and quasi-interpolation using Gaussians**

**Jeremy Levesley** *(University of Leicester)*

Sparse grid approximation provides a technique for approximation of functions in moderate dimensions, 5-10, say. In this talk we will discuss sparse approximation with smooth kernels, which give potential for faster than polynomial convergence for smooth input. We describe both interpolation and quasi-interpolation and describe multi-level versions of these algorithms.

**Parallel eigensolvers for electronic structure computations**

**Antoine Levitt** *(Universite Pierre et Marie Curie, France)*

Density functional theory (DFT) aims to solve the Schrödinger equation by modelling electronic correlation as a function of density. Its relatively modest $O(N^3)$ scaling makes it the standard method in electronic structure computation for condensed phases containing up to thousands of atoms. Computationally, its bottleneck is the partial diagonalisation of a Hamiltonian operator, which is usually not formed explicitly.

Using the example of the Abinit code, I will discuss the challenges involved in scaling plane-wave DFT computations to petascale supercomputers, and show how the implementation of a new method results in good parallel behaviour up to tens of thousands of processors. I will also discuss some open problems in the numerical analysis of eigensolvers and extrapolation methods used to accelerate the convergence of fixed point iterations.

## Minisymposium M6

## Recent advances in numerical methods for hyperbolic conservation laws

Organiser
Tristan Pryer

### Conservation Based Moving-Mesh Methods for Conservation Laws

**N. Arthurs,** M. Baines, T. Pryer & P. Sweby *(University of Reading)*

Hyperbolic Conservation laws arise in many areas of physics such as fluid dynamics and traffic flow. The existence of shocks within entropy solutions to conservation laws leads to a need for mesh refinement for an accurate solution. We present an $r$-refinement method for numerically solving conservation laws and show how such methods may be analysed. The method relies on local conservation to determine the velocity of nodes and is derived from the Lagrangian formulation of the PDE.

### Entropy based error estimates for fully discrete schemes for hyperbolic conservation laws

**Jan Giesselmann** & Andreas Dedner *(University of Stuttgart)*

This talk is concerned with nonlinear systems of hyperbolic conservation laws

$$\partial_t \mathbf{u} + \nabla \cdot (\mathbf{f}(\mathbf{u})) = 0 \qquad (1)$$

endowed with a strictly convex entropy/entropy flux pair and their numerical approximation via Runge-Kutta discontinuous Galerkin schemes. We are particularly interested in the derivation of a posteriori error estimates. Their derivation is based on combining a reconstruction approach with the relative entropy stability framework. The idea of reconstruction, in this context, is to compute a Lipschitz continuous function $\hat{\mathbf{u}}$ from the numerical solution $\mathbf{u}_h$ such that the residual

$$\mathcal{R} := \partial_t \hat{\mathbf{u}} + \nabla \cdot (\mathbf{f}(\hat{\mathbf{u}}))$$

is computable. Then, the relative entropy can be used to bound the difference between $\hat{\mathbf{u}}$ and the exact (entropy) solution $\mathbf{u}$ of (1) in terms of $\mathcal{R}$. Reconstructions for spatially semi-discrete schemes in one space dimension have been suggested in previous works. The focus of this talk is reconstruction in time allowing for numerical solutions obtained by explicit Runge-Kutta time integration schemes.

### Multi-level Monte-Carlo methods for entropy measure valued solutions of hyperbolic conservation laws

**Kjetil Olsen Lye** & Siddhartha Mishra *(ETH Zurich)*

A major difficulty in the theory of multi-dimensional systems of conservation laws is the question of well-posedness. In a recent paper, Fjordholm et al [1] advocated that the notion of an entropy measure valued solution (EMVS), is a suitable notion of solution for multi-dimensional systems. In the same paper, a numerical framework for computing the EMVS was developed using Monte-Carlo sampling.

We briefly review the theory of entropy measure valued solutions. We show how the numerical framework can be improved by utilizing Multi-level Monte-Carlo (MLMC) approximations, obtaining a speedup compared to the previously proposed Monte-Carlo sampling procedure, even in the setting where we do not have convergence of single samples. We show numerical experiments using the Euler equations with unstable initial data, and compare the MLMC method with the traditional MC method for EMVS.

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### Embedded Boundary Methods for flow in complex geometries

**Sandra May** & Marsha Berger *(ETH Zurich, New*

*York University)*

Cut cells methods have been developed in recent years for computing flow around bodies with complicated geometries. They are an alternative to body fitted or unstructured grids, which may be harder to generate and more complex in the bulk of the flowfield. Cut cell methods "cut" the flow body out of a regular Cartesian grid. Most of the grid is regular. Special methods must be developed for the "cut cells", which are cells that intersect the boundary. Cut cells can have irregular shapes and may be very small.

We present a mixed explicit implicit time stepping scheme for solving the advection equation on a cut cell mesh. The scheme represents a new approach for overcoming the small cell problem: namely, that explicit time stepping schemes are not stable on the arbitrarily small cut cells. Instead, we use an implicit scheme near the embedded boundary, and couple it to a standard explicit scheme used over most of the mesh. We compare several ways of coupling the explicit and implicit scheme, and prove a TVD result for one of them, which we call "flux bounding". We present numerical results in one and more dimensions. These results show second-order accuracy in the $L^1$ norm and between first- and second-order accuracy in the $L^\infty$ norm.

**Optimal error estimates for discontinuous Galerkin methods based on upwind-biased fluxes for linear hyperbolic equations**

**Xiong Meng** & Chi-Wang Shu, Boying Wu *(University of East Anglia)*

In this talk, we analyze discontinuous Galerkin methods using upwind-biased numerical fluxes for time-dependent linear conservation laws. In one dimension, optimal a priori error estimates of order $k+1$ are obtained when piecewise polynomials of degree at most $k$ ($k \geq 0$) are used. Our analysis is valid for arbitrary nonuniform regular meshes and for both periodic boundary conditions and for initial-boundary value problems. We extend the analysis to the multi-dimensional case on Cartesian meshes when piecewise tensor product polynomials are used. Numerical experiments are shown to demonstrate the theoretical results.

**Smoothness-Increasing Accuracy-Conserving (SIAC) Filtering for Discontinuous Galerkin Solutions over Nonuniform Meshes: Superconvergence and Optimal Accuracy**

Xiaozhou Li *(Delft University of Technology)* & **Jennifer K. Ryan** *(University of East Anglia)*

Smoothness-Increasing Accuracy-Conserving (SIAC) filtering is an area of rising interests in view of the fact that it can extract the hidden accuracy in discontinuous Galerkin (DG) solutions. It has been proven that by applying the SIAC filter to a DG solution, the accuracy order of the DG solution is raised from order $k+1$ to order $2k+1$ for linear hyperbolic equations over uniform meshes. However, applying the SIAC filter over nonuniform meshes is challenging and the quality of filtered solutions is usually dissatisfactory. The applicability for handling nonuniform meshes has already become the biggest obstacle to the development of SIAC filter. In this talk we discuss a relation between the filtered solutions and the unstructuredness of nonuniform meshes. Further, we demonstrate that there exists an optimal accuracy of the filtered solution for a given nonuniform mesh, and it is possible to approximate the optimal accuracy by designing an appropriate filter scaling. By applying the new designed SIAC filter over nonuniform meshes, the filtered solution has improved accuracy order as well as improved quality of the numerical solution.

**Convergence of a numerical scheme for a mixed hyperbolic-parabolic system in two space dimensions**

**Veronika Schleper** & Elena Rossi *(University of Stuttgart)*

We discuss the convergence of a numerical scheme for a mixed hyperbolic-parabolic system, modeling the behaviour of predators and preys, given by

$$\begin{aligned} &\partial_t u + div(f(u)v(w)) = (\alpha w - \beta)u \\ &\partial_t w - \mu\Delta w = (\gamma - \delta u)w \\ &v(w) = v(\eta * w) \\ &\qquad \text{for a sufficiently smooth kernel function } \eta \end{aligned} \tag{2}$$

This system is an extension of the classical Lotka-Volterra ordinary differential equations for predator prey systems that is able to include also the spatial variation of such systems. More precisely, we assume that the predators with density $u$ can feel the presence of preys in a (small) radius around them, such that the velocity field of predator propagation depends on a convolution of the prey density $w$ with a compactly supported kernel function $\eta$. Preys are assumed to diffuse independently of the predator density around them. The source terms account for birth and death of predators and preys respectively and are taken from the standard Lotka-Volterra equations.

The numerical scheme for (1) is obtained by a Lax-Friedrichs like finite volume discretization for the hyperbolic equation in combination with a standard ex-

plicit first order finite difference discretization for the parabolic equation. In both equations, the source terms are included by operator splitting, which allows a simple proof of positivity of $u$ and $w$.

After a short discussion of all relevant assumptions on the system parameters, we will focus on the modifications of the standard Lax-Friedrichs flux for (1) that allows us to obtain $L^1$-, $L^\infty$- and spatial $TV$-bounds for $u$ and $w$. Due to the parabolic character of the second equation in (1), no uniform $L^1$-Lipschitz continuity of $w$ in time can be expected. To obtain convergence of the scheme, we show how we can exploit the special structure of the hyperbolic part. Hereby, the convolution $\eta * w$ in the velocity field plays an important role to obtain strong convergence of $u$ in $L^1$, while—as a consequence of the missing $L^1$-Lipschitz continuity—convergence of $w$ can only be obtained weakly* in $L^\infty$.

To conclude the presentation, we show some numerical results that confirm the convergence in $L^1$ and show that system (1) yields solutions with the characteristic Lotka-Volterra structure.

### On the entropy dissipation of adaptive mesh reconstruction techniques

**Nikolaos Sfakianakis** & Maria Lukacova *(Johannes-Gutenberg University of Mainz)*

Classical methods for the analysis of adaptive mesh reconstruction (r-AMR) techniques address only the time evolution step of the procedure. To get though a deeper insight in the behaviour of r-AMR methods, the reconstruction of the mesh should also be taken into account.

To this end, we first present numerical evidence that indicate that r-AMR methods (and in particular the mesh reconstruction step) can have strong entropy stabilization properties, [3]. Further, we provide an analytical framework to study the entropy dissipation that a particular class of r-AMR exhibits, including the reconstruction of the mesh and the update of the solution, [1], [2].

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### A well-balanced kinetic scheme for the shallow water equations with rain

**Philip Townsend**, Mehmet Ersoy, & Omar Lakkis *(University of Sussex)*

The flow of water in rivers and oceans can, under certain assumptions, be efficiently modelled using the shallow water equations, a system of hyperbolic conservation laws which can be derived from a starting point of incompressible Navier-Stokes. Work by Perthame et al. in the late nineties developed a kinetic scheme for this hyperbolic system which can be shown to have certain desirable, well-balanced features. In flood risk assessment models, these properties are additionally desirable, but such a fully integrated model must account for the sources of flooding, an addition which no longer guarantees that such a kinetic scheme is applicable. We present here an extension of the standard shallow water system which incorporates an additional rain term on the surface of the water and infiltration of the water into the ground below, and show how this system can be modelled numerically through a careful extension of the formulation in the kinetic schemes mentioned above.

### Automated parameters for troubled-cell indicators using outlier detection

**Mathea J. Vuik** & Jennifer K. Ryan *(Delft University of Technology)*

In general, solutions of nonlinear hyperbolic PDE's contain shocks or develop discontinuities. One option for improving the numerical treatment of the spurious oscillations that occur near these artifacts is through the application of a limiter. The cells where such treatment is necessary are referred to as troubled cells, which are selected using a troubled-cell indicator. Examples are the KXRCF shock detector, the minmod-based TVB indicator, and the modified multiwavelet troubled-cell indicator.

The current troubled-cell indicators perform well as long as a suitable, problem-dependent parameter is chosen. An inappropriate choice of the parameter will result in detection of too few or too many elements. Detection of too few elements leads to spurious oscillations, since not enough elements are limited. If too many elements are detected, then the limiter is applied too often, and therefore the method is more costly and the approximation smooths out after a long time. The optimal parameter is chosen such that the

minimal number of troubled cells is detected and the resulting approximation is free of spurious oscillations. In general, many tests are required to obtain this optimal parameter for each problem.

In this presentation, we will see that the sudden increase or decrease of the indicator value with respect to the neighboring values is important for detection. Indication basically reduces to detecting the outliers of a vector (one dimension) or matrix (two dimensions). This is done using Tukey's boxplot approach to detect which coefficients in a vector are straying far beyond others [2].

We provide an algorithm that can be applied to various troubled-cell indication variables. Using this technique, the problem-dependent parameter that the original indicator requires, is no longer necessary, as the parameter will be chosen automatically.

We will apply this technique to the modified multiwavelet troubled-cell indicator [3, 4], which can be used to detect discontinuities in (the derivatives of) the DG approximation. Here, Alpert's multiwavelet basis is used [1]. We will use either the original indicator (with an optimal parameter), or the outlier-detection technique. In that way, the performance of the new technique can be easily compared to the current method.

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## Minisymposium M7

## Chebfun: new developments cool applications and on the horizon

Organiser
Nick Trefethen

**Krylov methods for operators**

**Jared L. Aurentz** *(University of Oxford)*

In this talk we will explore the convergence of Krylov methods when used to solve $Lu = f$ where $L$ is an unbounded linear operator. We will show that for certain problems, methods like Conjugate Gradients and GMRES still converge even though the spectrum of $L$ is unbounded. A theoretical justification for this behavior is given in terms of polynomial approximation on unbounded domains.

**High-Accuracy Chebyshev Coefficients via Contour Integrals**

**Anthony Austin** *(University of Oxford)*

Following Bornemann's work on computing Taylor coefficients to high precision by contour integrals over circles of large radius, Wang and Huybrechs have recently published a paper about computing Chebyshev coefficients to high precision by contour integrals over Bernstein ellipses of large parameter. Under certain circumstances, these methods make it possible to compute coefficients in ordinary floating-point arithmetic down at the level of $10^{-100}$ or below. We investigate the use of such methods for general-purpose computation with functions as in Chebfun.

**Computing distinct solutions of nonlinear ODEs with Chebfun**

**Asgeir Birkisson** *(University of Oxford)*

Like nonlinear system of equations, nonlinear differential equations may permit several nontrivial distinct solutions. This talk describes how distinct solutions of nonlinear boundary-value problems can be computed in Chebfun. The first technique presented is called *deflation*, which modifies the residual of the original differential equation, so that Newton's method no longer converges to currently known roots. The second technique discussed is path-following, where the introduction of a continuation parameter enables tracing curves in solution spaces to yield further solutions, starting from a previously known solution.

**From 2D to 3D**

**Behnam Hashemi** *(University of Oxford)*

Let $f : [a, b] \times [c, d] \times [e, g] \to \mathbb{C}$ be a trivariate continuous function. If $f$ is sufficiently smooth then it has a trivariate Chebyshev expansion

$$f(x, y, z) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} c_{ijk} T_k(z) T_j(y) T_i(x).$$

In this talk, we show how to create chebfun3 objects in different ways. The first approach is an automatic

tensor technique that relies on 1D Chebyshev mathematics only. This is implemented in the new "chebfun3t" class. Given a smooth trivariate function $f$, it computes an order-3 tensor containing coefficients of the Chebyshev expansion of $f$. The second approach is based on low-rank approximations which is the idea behind Chebfun2. This is implemented in the new "chebfun3" class and creates what we call a "slice decomposition" of $f$. We discuss a few other methods, describe some details of our current implementations, try to compare the approaches and summarize challenges ahead.

**Analytic continuation, phase portraits, and the zeta function**

**Mohsin Javed** *(University of Oxford)*

The aim of this talk is to learn something new about analytic continuation via numerical experiments. Using Chebfun, we will interpolate the Riemann zeta function on a vertical line segment in the half plane $z > 1$ and then find and compare the roots of this interpolant with the roots of the zeta function. Similar numerical experiments for rational interpolants of the zeta function will also be discussed. We will also talk about phase portraits and how they help us visualize analytic functions in the complex plane.

**Computing choreographies**

**Hadrien Montanelli** & Nikola I. Gushterov *(University of Oxford)*

Choreographies are periodic solutions of the $n$-body problem in which all of the bodies have unit masses, share a common orbit and are uniformly spread along it. In this talk, I will present an algorithm for numerical computation of choreographies in the plane in a Newtonian potential and on the sphere in a cotangent potential. It is based on stereographic projection, approximations by trigonometric polynomials, minimization of the action functional using a closed-form expression for the gradient and quasi-Newton methods.

**A fast and well-conditioned spectral method for singular integral equations**

**Richard Mikaël Slevinsky** *(University of Oxford)* & Sheehan Olver *(The University of Sydney)*

We develop a spectral method for solving univariate singular integral equations over unions of intervals and circles, by utilizing Chebyshev, ultraspherical and Laurent polynomials to reformulate the equations as banded infinite-dimensional systems. Low rank approximations are used for efficient representations of the bivariate kernels. The resulting system can be solved in $O(n^{\text{opt}})$ operations using an adaptive QR factorization, where $n^{\text{opt}}$ is the optimal number of unknowns needed to resolve the true solution. Applications considered include fracture mechanics, the Faraday cage, and acoustic scattering. The Julia software package `SIE.jl` implements our method with a convenient, user-friendly interface.

**Initial value problems and a new ODE textbook**

**Nick Trefethen** *(University of Oxford)*

ODEs are generally either initial-value or boundary-value problems, and both the behaviour and the appropriate numerical methods differ greatly. In the past year, however, Asgeir Birkisson has modified Chebfun so that it solves both kinds of problems by a unified syntax: to solve a linear or nonlinear problem $L(u) = f$ together with initial or boundary conditions, one can type `u = L\f`. The underlying algorithms involve automatic Chebyshev spectral discretization for BVPs and marching via ODE113 for IVPs. Taking advantage of this framework, a new textbook is about half-drafted whose subject is ODEs, not numerics, even though illustrations enabled by numerics appear on every page. The current draft opening sentence is "What if all you had to do to solve an ODE were just to write it down?"

## Minisymposium M8

## Data Analytics and Uncertainty Quantification

Organisers

Des Higham and Alistair Forbes

**Probability Measures on Numerical Solutions of ODEs and PDEs for Uncertainty Quantification and Inference**

**Patrick Conrad**, Mark Girolami & Andrew Stuart *(University of Warwick)*, Konstantinos Zygalakis *(University of Southampton)* & Simo Särkkä *(Aalto University)*

Deterministic ODE and PDE solvers are widely used, but characterizing the error in numerical solutions within a coherent statistical framework is challenging. We successfully address this problem by constructing a probability measure over functions

consistent with the solution that provably contracts to a Dirac measure on the unique solution at rates determined by an underlying deterministic solver. The measure straightforwardly derives from important classes of numerical solvers and is illustrated on uncertainty quantification and inverse problems

**A practical method to assess parameter sensitivity and uncertainty in C-cycle models**

**S. Delahaies** & I. Roulstone, N. Nichols*(University of Surrey)*

The carbon cycle combines multiple spatial and temporal scales, from minutes to hours for the chemical processes occurring in plant cells to several hundred of years for the exchange between the atmosphere and the deep ocean and finally to millennia for the formation of fossil fuels. Together with our knowledge of the transformation processes involved in the carbon cycle, many Earth Observation systems are now available to help improving models and predictions using inverse modelling techniques. A generic inverse problem consists in finding a $n$-dimensional state vector $x$ such that

$$h(x) = y, \tag{1}$$

for a given $N$-dimensional observation vector $y$, including random noise, and a given model $h$. The problem is well posed if the three following conditions hold: 1) there exists a solution, 2) the solution is unique and 3) the solution depends continuously on the input data. If at least one of these conditions is violated the problem is said to be ill-posed. The inverse problem (1) is often ill-posed, a regularization method is required to replace the original problem with a well posed problem and solving (1) amounts to 1) constructing a solution x, 2) assessing the validity of the solution, 3) characterizing its uncertainty.

The data assimilation linked ecosystem carbon (DALEC) model is a simple box model simulating the carbon budget allocation for terrestrial ecosystems. Intercomparison experiments have demonstrated the relative merit of various inverse modelling strategies (MCMC, ENKF) to estimate model parameters and initial carbon stocks for DALEC using eddy covariance measurements of net ecosystem exchange of CO2 and leaf area index observations. Most results agreed on the fact that parameters and initial stocks directly related to fast processes were best estimated with narrow confidence intervals, whereas those related to slow processes were poorly estimated with very large uncertainties. While other studies have tried to overcome this difficulty by adding complementary data streams or by considering longer observation windows no systematic analysis has been carried out so far to explain the large differences among results.

We consider adjoint based methods to investigate inverse problems using DALEC and various data streams. Using resolution matrices we study the nature of the inverse problems (solution existence, uniqueness and stability) and show how standard regularization techniques affect resolution and stability properties. We then use ecological common sense and constrained optimization techniques to constrain the parameter space. This approach, rapid and efficient, allows us to compute ensembles of solutions to the model-data fusion problem from which robustness of the variational method can be established and parameter distributions can be obtained.

**Accounting for model inadequacy in environmental monitoring**

**Alistair Forbes** *(National Physical Laboratory)*

Much of environmental monitoring involves establishing trends in environmental variables such as atmospheric composition or levels of air pollution from measured data. The data records generally show approximately cyclical annual and diurnal variation, as well as short term variation and an underlying baseline drift. Often, data is missing over randomly spaced time intervals. The data will also reflect instrument effects, including instrument drift. For the most part, there will be no physical theory that is able to predict the form of the baseline drift or departure from periodic behaviour of the annual and diurnal variations. Empirical models such as polynomials or Fourier series can be used but any choice of an empirical model is likely to imply that we have more knowledge about the physical system than is warranted.

There are a number of ways of addressing the likely inadequacy of a given empirical model. A model selection approach is to consider all plausible models and then choose the best one using some criterion, such as the Akaike Information Criterion or the Bayes Information Criterion, that balances the goodness of fit with compactness of representation. A model averaging approach, rather then selecting one from all the competing models, provides a weighted average of all the models where the weighting reflects how well a model is supported by the data [4]. A third approach is to augment a basic empirical model capturing the main response features by a statistical effects model obeying spatial and/or temporal correlation [3]. The degree of correlation controls the effective number degrees of freedom [2] associated with the model – the higher the correlation, the lower the number of degrees of freedom. For linear models, the fitted data vector $\hat{\boldsymbol{y}} = S\boldsymbol{y}$ is a linear mapping of the data vector $\boldsymbol{y}$ by

the smoothing matrix $S$. The effective number of degrees of freedom is the sum of the eigenvalues of this matrix. The statistical effects model essentially adds a new degree of freedom for each data point while the correlation provides prior information (or a regularisation term) that reduces the number of degrees of freedom. Often, the statistical effects model can be re-interpreted as an empirical model with an appropriate number of degrees of freedom and having the same correlation behaviour, leading to significant savings in computational expense [1].

This talk will discuss such models and corresponding algorithms in applications relating to monitoring atmospheric oxygen concentration and air quality.

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**Parameter estimation for the stochastic SIS epidemic model**

**Alison Gray** & Jiafeng Pan, David Greenhalgh, Xuerong Mao *(University of Strathclyde)*

In this work [1] we estimate the parameters in the stochastic SIS (susceptible-infected-susceptible) epidemic model [2] by using pseudo-maximum likelihood estimation (pseudo-MLE) and least squares estimation. We obtain the point estimators and $100(1-\alpha)\%$ confidence intervals as well as $100(1-\alpha)\%$ joint confidence regions by applying least squares techniques. The pseudo-MLEs have almost the same form as the least squares case. We also obtain the exact as well as the asymptotic $100(1-\alpha)\%$ joint confidence regions for the pseudo-MLEs. Computer simulations are used to illustrate our theory.

**References**

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**Message-Passing Hierarchy in a Dynamic Network**

**Alexander V. Mantzaris** & Desmond J. Higham *(University of Strathclyde)*

Messages may follow preferred directions over time in online communication networks. There are many possible explanations for this asymmetric flow of information. For example, some members may have better access to information that relates to the whole network or there may be an imposed chain of command. We assume the latter scenario; i.e., there is a ranking amongst the nodes which biases the direction of information flow. An algorithm to quantify the level of such bias will be derived and illustrated. Key applications are (a) to discover hidden hierarchical structure when it has not been specified, and (b) to quantify whether individual nodes are respecting a known hierarchical ordering.

**Efficient solvers for unsteady incompressible flow: hydrodynamic stability and UQ**

**David Silvester** *(University of Manchester)*

This talk highlights some recent developments in the design of robust solution methods for the Navier-Stokes equations modelling incompressible fluid flow. Our focus is on uncertainty quantification. We discuss stochastic collocation approximation of critical eigenvalues of the linearised operator associated with the transition from steady flow in a channel to vortex shedding behind an obstacle. Our computational results confirm that classical linear stability analysis is an effective way of assessing the stability of such a flow.

## Minisymposium M9

## Numerical methods for fractional differential equations

Organisers
Yanghong Huang and Bangti Jin

**High-Order Accurate Local Schemes for Fractional Differential Equations**

**Daniel Baffet** & Jan Hesthaven *(EPFL)*

In this talk we discuss high-order methods for fractional differential equations of the form $D^\alpha u = f(u,t)$, where $D^\alpha$ is the Caputo $\alpha$-derivative, and $0 < \alpha < 1$. The proposed methods are inspired by the high-order multi-step Adams methods. To approximate the history term, we use an expansion in some weighted $L^2$ space. In practice, the expansion is truncated, and only a finite number of terms is retained. The coefficients of this expansion are considered as auxiliary variables of the scheme and are advanced in time during the time-stepping procedure. To overcome possible singularities at the initial time, as well as to increase the scheme's efficiency, we have implemented an adaptive step-size method. Building on estimates of the truncation error, we adapt the Milne device to the current problem and employ it as an error indicator. The performance of some schemes is illustrated numerically.

**Modelling and simulating the electrophysiology of a heterogeneous human heart by fractional models**

**Kevin Burrage** *(University of Oxford, UK and Queensland University of Technology, Australia)*

In this presentation I discuss how we can use non-local (space fractional) models to model the electrophysiology of the heart. I give sound justifications based on potential theory for using these models in a bi-domain formulation and then develop some new efficient computational techniques based on spectral techniques.

Finally I describe how these fractional models can be calibrated from diffusion tensor imaging data and discuss their relevance for understanding the structural heterogeneities of the human heart and their roles on cardiac electrophysiology.

This is joint work with Blanca Rodriguez, Alfonso Bueno-Orovio and Vicente Grau (Oxford)

**Finite difference methods for fractional Laplacian**

**Yanghong Huang** *(Imperial College London)*

The fractional Laplacian is the prototypical example of non-local diffusion, and has been employed in many models with long range interactions. In this talk, a general form of the finite difference scheme is proposed and several existing methods in one dimension are reviewed or derived. The general form of the scheme has many discrete counterparts of its continuous definition: discrete convolution, random walk, and multiplier (or symbol) in semi-discrete Fourier transform. Despite the non-locality, the accuracy of different schemes can be obtained from the symbol, and is verified numerically. The schemes are also compared under different criteria, and can be chosen according to the applications. This is a joint work with Adam Oberman in McGill University.

**Variational formulation of problems involving fractional order differential operators**

**Bangti Jin** *(University College London)*

In this talk, we consider boundary value problems involving either Caputo or Riemann-Liouville fractional derivatives of order $\alpha \in (1,2)$ on the unit interval $(0,1)$. The variational problem for the Riemann-Liouville case is coercive on the space $H^{\alpha/2}$ but the solutions are less regular, whereas that for the Caputo case involves different test and trial spaces. We establish the regularity pickup of the solutions of the variational problem, which enables one to establish convergence rates of the finite element approximations. Finally, numerical results are presented to illustrate the error estimates.

**Numerical methods for some linear stochastic space-fractional partial differential equations**

**Monzorul Khan** *(University of Chester)* & Fang Liu *(Lvliang University, P.R. China)* & Yubin Yan *(University of Chester)*

Fourier spectral methods for solving some linear stochastic space-fractional partial differential equations perturbed by space-time white noises in a one-dimensional case are introduced and analyzed. The space-fractional derivative is defined by using the eigenvalues and eigenfunctions of Laplacian subject to some boundary conditions. We approximate the space-time white noise by using piecewise constant functions and obtain the approximated stochastic space-fractional partial differential equations. The approximated stochastic space-fractional partial differential equations are then solved by using Fourier spectral methods. Error estimates in $L^2$- norm are obtained.

**Higher order Grünwald approximations of fractional derivatives and fractional powers of operators**

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

We give stability and consistency results for higher order Grünwald-type formulae used in the approximation of solutions to fractional-in-space partial dif-

ferential equations. We use a Carlson-type inequality for periodic Fourier multipliers to gain regularity and stability results. We then generalise the theory to the case where the first derivative operator is replaced by the generator of a bounded group on an arbitrary Banach space.

**Higher order numerical methods for solving fractional differential equations**

**Kamal Pal** & Yubin Yan and & N. J. Ford *(University of Chester)*

In this talk we introduce higher order numerical methods for solving fractional differential equations. We use two approaches to consider this problem. One approach is based on a direct discretization of the fractional differential operator and we obtain a numerical method for solving a linear fractional differential equation with order $0 < \alpha < 1$. The order of convergence of the numerical method is $O(h^{3-\alpha})$. Another approach is based on the discretization of the integral in the equivalent form of the fractional differential equation and we obtain a fractional Adams-type method for the nonlinear fractional differential equation with any order $\alpha > 0$. The order of convergence of the numerical method is $O(h^3)$ for $\alpha \geq 1$ and $O(h^{1+2\alpha})$ for $0 < \alpha \leq 1$ for sufficiently smooth solutions. The numerical examples are given to show that the numerical results are consistent with the theoretical results.

**Solution of Caputo and Riemann-Liouville two-point boundary value problems by reformulations using weakly singular Volterra integral equations**

**Martin Stynes** & Natalia Kopteva *(Beijing Computational Science Research Center)*

Two-point boundary value problems of the form $D^\mu u + bu' + cu = f$ are considered with appropriate boundary conditions; here $D^\mu$ is a fractional differential operator of order $\mu$ (with $1 < \mu < 2$) that can be of Caputo or Riemann-Liouville type. Simple examples show that low-order derivatives of the solutions to these problems typically blow up at one endpoint of the interval, but until now a general theory for this behaviour has been lacking in the Riemann-Liouville case. Here both classes of boundary value problem are analysed (i.e., existence, uniqueness, and sharp pointwise bounds on the derivatives of $u$ are proved rigorously) by a reformulation of each problem based on weakly singular Volterra integral equations of the second kind which are then solved by piecewise-polynomial collocation methods, for which sharp error bounds are derived. The exact reformulation chosen depends critically on the type of fractional derivative involved.

**Error estimates of finite element method for linear space-fractional partial differential equations**

**Yubin Yan** *(University of Chester)* & Fang Liu *(Lvliang University, P. R. China)* & Monzorul Khan *(University of Chester)*

Finite element methods for solving linear space-fractional partial differential equations are considered in a one-dimensional case. The space-fractional derivative is defined as a Riesz fractional derivative. The $L^2$-norm error estimates in the semidiscrete case are proved by two different methods and the error bounds depend on the regularities of the exact solutions of the space-fractional partial differential equations. One method is by using a duality argument and the error bounds contain the norm $\|u_t\|_{L^2(0,1)}$ of the time derivative of the exact solution. Another method is by using the approximate solution operator of the corresponding fractional elliptic problem and the error bounds contain the norm $\|u_t\|_{H_0^\alpha(0,1)}, 1/2 < \alpha \leq 1$ of the time derivative of the exact solution.

## Minisymposium M10

## Numerical methods for feedback control of dynamical systems and related topics

Organiser
Dante Kalise

**Uncertainty Quantification in Control Problems for Flocking Models**

**G. Albi** *(TU München, Germany)*, L. Pareschi & M. Zanella *(University of Ferrara, Italy)*

In this talk the optimal control of flocking models with random inputs is investigated from a numerical point of view. We consider a system of agents governed by a Cucker-Smale type model, where the effect of uncertainty is included in the interaction kernel. Using a generalized polynomial chaos (gPC) approach we analyse the influence of random parameters on the system, showing analytical and numerical threshold effects in the alignment dynamic. A selective model predictive control approach is used in order to enforce and stabilize the system, even in unstable regimes, and to steer the whole ensemble of agents towards a desired direction.

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### Sparse Control of Alignment Models in High Dimension

**Mattia Bongini** & Massimo Fornasier & Oliver Junge & Benjamin Scharf *(Technische Universität München)*

Dynamical systems of Cucker-Smale type can be used to describe the pattern formation of multi-agent dynamical systems. In this context, two situations may arise: if the difference between the velocities of the agents is not too large in comparison to the distances of the agents, the system tends autonomously to consensus. Otherwise, when there is no self-organization, it was shown recently that an external policy maker can steer the system to consensus using a sparse control acting only on the agent farthest away from the mean velocity. However, in real-life situations, the dimension of the agents might be very large (for instance, consider portfolios' dynamics in the stock market) and numerical simulations of this kind of control problem can be totally unfeasible due to the curse of dimensionality, even if the number of agents is very small. In this talk we will present a possible solution to this problem based on Johnson-Lindenstrauss embeddings to reduce the dimensionality of the dynamical system. We show that we can choose the agent on which we want to exert control in high dimension to steer the system to consensus only by using the information from the low-dimensional one. Hence, it is sufficient to simulate the projected system to compute an effective strategy for the high-dimensional control problem. Quite surprisingly, the reduction of the dimensionality can be even of the order of 90% of the original dimension, thus saving an enormous amount of computational time.

### Reconstruction of independent sub-domains for a class of Hamilton-Jacobi equations and application to parallel computing

**Adriano Festa** *(RICAM - Austrian Academy of Sciences)*

A previous knowledge of the domains of dependence of a Hamilton-Jacobi equation can be useful in its study and approximation. Information of this nature is, in general, difficult to obtain directly from the data of the problem. In this talk we introduce formally the concept of *independent sub-domain* discussing its main properties and we provide a constructive implicit representation formula. Using such results we propose an algorithm for the approximation of these sets that is shown to be relevant in the numerical resolution via parallel computing.

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### Model Predictive Control of stochastic processes via the Fokker-Planck Equation

**A. Fleig** & L. Grüne, R. Guglielmi *(University of Bayreuth)*

Optimal control of a stochastic process that is modelled by an Itô stochastic differential equation can often be achieved via controlling the underlying probability density function (PDF). Its time evolution is prescribed by the Fokker-Planck equation, a second order parabolic PDE. In this manner, the original problem can be reformulated as a PDE-constrained optimisation problem.

In this talk, a Model Predictive Control scheme is applied in order to track the solution of the Fokker-Planck equation over a fixed time interval. The control, while being piecewise constant in time, may also depend on space, resulting in a feedback loop when applying the control strategy directly to the stochastic process. We compare the results obtained by a space-dependent control function to space-independent control and analyse the dependence of the MPC algorithm on the prediction horizon and the sampling time. In addition, we present numerical simulations of stochastic processes with the computed control strategy applied directly to the process.

### High-order schemes for static Hamilton-Jacobi-Bellman equations

**Dante Kalise** *(Radon Institute for Computational and Applied Mathematics, Linz, Austria)*

A standard tool for the solution of optimal control problems is the application of the Dynamic Programming Principle proposed by Bellman in the 50's. In this context, the value function of the optimal control problem is characterized as the viscosity solution of a first-order and fully nonlinear Hamilton-Jacobi-Bellman (HJB) equation. A major advantage of the approach is the existence of a feedback mapping con-

necting the current state of the system and the associated optimal control. In this talk, we present a high-order semi-Lagrangian scheme for the approximation of stationary HJB equations. The resulting nonlinear discrete system is solved via a fixed point approximation scheme. The convergence of the fixed point operator is justified by an $\epsilon$-monotonicity argument.

### DGFEM approximation of parabolic HJB equations with Cordes coefficients

**Iain Smears** & Endre Süli *University of Oxford*

We will present theoretical and computational aspects of the *hp*-version DGFEM for fully nonlinear second-order parabolic Hamilton–Jacobi–Bellman (HJB) equations of the form

$$\begin{aligned} \partial_t u - \sup_{\alpha\in\Lambda}[L^\alpha u - f^\alpha] = 0 \quad &\text{in } \Omega\times(0,T), \\ u = 0 \quad &\text{on } \partial\Omega\times(0,T), \\ u = u_0 \quad &\text{on } \Omega\times\{0\}, \end{aligned} \tag{1}$$

where, for each $\alpha\in\Lambda$, $L^\alpha = a^\alpha : D^2 + b^\alpha\cdot\nabla - c^\alpha$ is a uniformly elliptic operator. We consider the class of HJB equations that satisfy the Cordes condition: the Cordes condition: there exist $\varepsilon\in(0,1]$, $\lambda>0$ and $\omega>0$ such that

$$\frac{|a^\alpha|^2+1/\lambda^2+1/\omega^2}{(\mathrm{Tr}\,a^\alpha+1/\lambda+1/\omega)^2} \le \frac{1}{d+1+\varepsilon} \quad \text{in } \overline{\Omega}\times[0,T], \ \forall\,\alpha\in\Lambda. \tag{2}$$

The discretisation of the PDE is motivated by a continuous analysis based on the Cordes condition, which establishes well-posedness in the class of strong solutions. The numerical scheme is obtained by combining a nonstandard discontinuous Galerkin time-stepping scheme with the spatial discretisation of HJB equations from our earlier works [1, 2]. The time-stepping scheme is unconditionally stable for arbitrary time-step lengths and for arbitrary approximation orders.

The resulting method is then consistent and stable in a discrete $L^2(H^2(\Omega))\cap H^1(L^2(\Omega))$-type Bochner norm. For instance, when employing quasi-uniform meshes and uniform polynomial degrees $p$ in space, and uniform time steps $\tau$ with uniform temporal polynomial degree $q$ in time, the error bound is of the form

$$\begin{aligned} \|u-u_h\| \lesssim{}& \frac{h^{\min(s,\,p+1)-2}}{p^{s-7/2}}\|u\|_{L^2(H^s(\Omega))} \\ &+\frac{h^{\min(\bar{s},\,p+1)}}{p^{\bar{s}}}\|u\|_{H^1(H^{\bar{s}}(\Omega))} \\ &+\frac{h^{\min(\tilde{s},\,p+1)-1}}{p^{\tilde{s}-3/2}}\|u(0)\|_{H^{\tilde{s}}(\Omega)} + p^{3/2} \\ &\sum_{\ell\in\{0,2\}}\frac{\tau^{\min(\sigma_\ell,\,q+1)-1+\ell/2}}{q^{\sigma_\ell-1+\ell/2}}\|u\|_{H^{\sigma_\ell}(H^\ell(\Omega))}, \end{aligned} \tag{3}$$

where $\|\cdot\|$ denotes a discrete $L^2(H^2(\Omega))\cap H^1(L^2(\Omega))$-type norm over $(0,T)$, and where we assume that $s>5/2$, $\bar{s}>0$, $\tilde{s}>3/2$, and $\sigma_\ell\ge 1$ for $\ell\in\{0,2\}$. We will further present error bounds for solutions with lower regularity, as well as numerical experiments on strongly anisotropic problems.

### References

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[2] I. Smears and E. Süli, *Discontinuous Galerkin finite element approximation of Hamilton–Jacobi–Bellman equations with Cordes coefficients*, SIAM J. Numer. Anal., 52 (2014), pp. 993–1016.

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## Minisymposium M11

## Numerical linear algebra for optimisation and data assimilation

Organisers
Melina Freitag and John Pearson

### Simultaneous Random and Optimized Sources and Detectors for Efficient Optimization in Inverse Problems

**Eric de Sturler** ***(Virginia Tech)*** & Selin Sariaydin *(Virginia Tech)* & Misha Kilmer *(Tufts University)* & Serkan Gugercin *(Virginia Tech)*

In nonlinear inverse problems, we often optimize an objective function involving many right hand sides (corresponding to many measurements), where each system corresponds to solving a 3D PDE. This leads to the solution of a very large number of large linear systems for each nonlinear function evaluation, and potentially additional systems for evaluating or approximating Jacobians. We propose a combination of simultaneous random sources and detectors and optimized (for the problem) sources and detectors to drastically reduce the number of systems to be solved. We apply our approach to problems in diffuse optical tomography. Time permitting we will also report fast implementations on GPUs.

### Preconditioners for two-sided eigenvalue problems

**Melina A Freitag** *(University of Bath)*

Convergence results are provided for inexact two-sided inverse and Rayleigh quotient iteration. Moreover, the simultaneous solution of the forward and adjoint problem arising in two-sided methods is considered and the successful tuning strategy for preconditioners is extended to two-sided methods.

This is joint work with Patrick Kuerschner (MPI Magdeburg, Germany).

### Preconditioners for higher order methods in big data optimization

**Jacek Gondzio** & Kimonas Fountoulakis *(University of Edinburgh)*

We address efficient preconditioning techniques for the second-order methods applied to solve various sparse approximation problems arising in big data optimization. The preconditioners cleverly exploit special features of such problems and cluster the spectrum of eigenvalues around one. The inexact Newton Conjugate Gradient method excels in these conditions. Numerical results of solving L1-regularization problems of unprecedented sizes reaching a trillion of variables will be presented.

### References

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### Block Interface Preconditioners for Optimal Control of Elliptic PDE

**Daniel Loghin** *(University of Birmingham)*

The discretization of optimal control of elliptic partial differential equations problems yields optimality conditions in the form of linear systems with a block structure. Correspondingly, when the solution method is a non-overlapping domain decomposition method, we need to solve interface problems which exhibit a block structure as well. It is therefore natural to consider block preconditioners acting on the interface variables for the acceleration of Krylov methods with substructuring preconditioners.

In this talk we describe a technique which employs a preconditioner block structure based on the fractional Sobolev norms corresponding to the domains of the boundary operators arising in the matrix interface problem, some of which may include a dependence on the control regularization parameter. We illustrate our approach on standard elliptic control problems. We present analysis which shows that the resulting iterative method converges independently of the size of the problem. We include numerical results which indicate that performance is also independent of the control regularization parameter and exhibits only a mild dependence on the number of the subdomains.

### Preconditioning for constrained optimization problems

**John Pearson** *(University of Kent)*

The rapid solution of optimization problems with constraints frequently requires the development of effective and robust iterative methods for large-scale matrix systems – these may arise from a 'one-shot' solution algorithm for the optimization problem, or when establishing Newton search directions within a nonlinear iteration.

In this talk we discuss recent developments in the construction of preconditioned iterative methods for such matrix systems, which are of saddle point form and contain additional block structures. We proceed using carefully chosen approximations of the $(1, 1)$-block and Schur complement.

The applications considered in this talk include optimization problems with PDE constraints (including important problems from optimal flow control and fractional differential equations), and interior point methods for solving related problems with additional inequality constraints. In each case numerical experiments demonstrate the potency of our preconditioning strategies.

### Null-space preconditioners for saddle point problems

**Jennifer Pestana** *(University of Manchester)* & Tyrone Rees *(STFC Rutherford Appleton Laboratory)*

Large sparse saddle point problems

$$\underbrace{\begin{pmatrix} A & B^T \\ B & 0 \end{pmatrix}}_{\mathcal{A}} \begin{pmatrix} \boldsymbol{x} \\ \boldsymbol{y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{f} \\ \boldsymbol{g} \end{pmatrix},$$

with $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{m\times n}$, $m \leq n$, $\boldsymbol{f} \in \mathbb{R}^n$, are often solved by preconditioned iterative methods. When $A$ is invertible, effective preconditioners based on the range-space factorization

$$\mathcal{A} = \begin{pmatrix} I & \\ BA^{-1} & I \end{pmatrix} \begin{pmatrix} A & \\ & -S \end{pmatrix} \begin{pmatrix} I & A^{-1}B^T \\ & I \end{pmatrix}$$

are often used.

Here we propose alternative preconditioners, based on a null-space factorization, that can be applied even when $A$ is singular. We examine the spectra of the preconditioned matrices, and show how to apply our block lower triangular preconditioner using a conjugate gradient method with a nonstandard inner product. We test the newly proposed preconditioners on a number of test cases from a range of applications.

**A multilevel preconditioner for data assimilation with 4D-Var**

**Alison Ramage** *(University of Strathclyde)*

Large-scale variational data assimilation problems are commonly found in applications like numerical weather prediction and oceanographic modelling. As part of the solution process, the 4D-Var method is frequently used to calculate a forecast model trajectory that best fits the available observations to within the observational error over a period of time. This results in a large-scale nonlinear weighted least-squares problem, typically solved by a Gauss-Newton method. One key difficulty is that the state vectors used in modern realistic data assimilation applications could contain billions or trillions of unknowns so, due to memory limitations, in practice it is often impossible to assemble, store or manipulate the matrices involved explicitly.

One way of addressing this problem is to use a limited memory approximation to the Hessian, computed using the Lanczos method, in the linearised quadratic minimisation subproblems. It is usually also necessary to further enhance the limited-memory algorithm by using an appropriate preconditioner: within this framework, it is standard to apply first-level preconditioning in the form of the square root of the background covariance matrix. However, if the impact of sensor information on the optimal solution is significant, this is not sufficient and an additional preconditioning step is required. In this talk, we will discuss using a multilevel approach as a "second-level" preconditioner within 4D-Var and investigate its usefulness in terms of reducing memory requirements and increasing computational efficiency.

This is joint work with Kirsty Brown (University of Strathclyde) and Igor Gejadze (IRSTEA, Montpellier).

**Observations on the use of block diagonal preconditioners with MINRES in interior point methods**

**Tyrone Rees** *(STFC Rutherford Appleton Laboratory)*

Primal-dual interior point methods have proved to be successful for solving quadratic programs of the form

$$\min \ \frac{1}{2}\mathbf{x}^T H\mathbf{x} + \mathbf{f}^T\mathbf{x}$$

$$\text{s.t. } B\mathbf{x} = \mathbf{g}, \quad \mathbf{x} \geq \mathbf{0}.$$

The main work in such an algorithm is in calculating a Newton-like search direction, which involves solving a family of equations of the form

$$\begin{bmatrix} H + S_k^{-1}X_k & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} \Delta\mathbf{x} \\ -\Delta\mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix}, \qquad (1)$$

where $S_k$ and $X_k$ are diagonal matrices that change as the iteration progresses. We are particularly interested in the case where $H$ and $B$ are sparse.

For sufficiently large systems sparse direct methods may fail to be effective on such problems, and in these cases it's natural to turn to iterative methods, and in particular Krylov subspace methods. However, such an approach requires us first to address two concerns:

1. As is typical in such a setting, we need to use an appropriate preconditioner in order to achieve satisfactory convergence.
2. Since we are solving to obtain a search direction, we must ensure that calculating this inexactly doesn't cause the outer interior point method to stagnate.

Chen Greif and Tim Rees [1] proposed solving the equation (1) using MINRES with an augmented Lagrangian preconditioner of the form

$$\mathcal{P} = \begin{bmatrix} H + S_k^{-1}X_k + B^TW^{-1}B & 0 \\ 0 & W \end{bmatrix}.$$

Greif and Rees, and more recently Morini, Simoncini and Tani [2], have derived spectral bounds that show that this is an effective preconditioner, answering the first of the points about. However, aside from showing

such a method works in practice, the second issue is not addressed.

In this talk I will show numerical tests that demonstrate the unreasonable effectiveness of MINRES with a block diagonal preconditioner, and give a theoretical underpinning to explain such behaviour.

**References**

[1] Rees, Tim, and Greif, Chen. "A preconditioner for linear systems arising from interior point optimization methods." SIAM Journal on Scientific Computing 29.5 (2007): 1992-2007.
[2] Morini, Benedetta, Simoncini, Valeria, and Tani, Mattia. "Unreduced symmetric KKT systems arising from interior point methods. part II: preconditioning." (2015, technical report)

**Simultaneous State and Parameter Estimation in Thermo-Elastic Models**

**Ilka Riedel** & Roland Herzog *(TU Chemnitz)*

We consider the thermo-elastic behaviour of machine tools. The goal is to estimate in real time the displacement at a certain point from few temperature measurements on the surface in a certain time window. Due to the uncertainty of some parameters, such as the heat transfer coefficient, it is necessary not only to estimate the temperature and displacement states but also these parameters to keep the model up-to-date in every time step.

To solve this problem of simultaneous state and parameter estimation we use self-calibrating data assimilation techniques. The use of parametric model order reduction techniques ensures the online capability of the method. Numerical examples are presented.

**Preconditioners for Optimization with Partial Integro-Differential Equations**

**Ekkehard W. Sachs** & Lukas Zimmer *(Trier University, Germany)*

In recent years, applications of optimization have become even more complex due to the nature of the physical problems. Among the well studied area of PDE (Partial Differential Equations) - constrained optimization the subarea of optimization with Partial Integro-Differential Equations (PIDE) has surfaced as a challenging research subject.

The applications in this field are numerous and interesting: they range from new models in material design, also called peridynamics, to applications in finance, i.e. models for pricing derivatives via jump-diffusion processes and even into biology for modeling cell adhesion processes.

The main difference between PDE and PIDE models is the occurrence of an integral term (here in the spatial coordinates) in the partial differential equation. This leads to a so-called non-local operator which has important consequences in the theoretical analyses but even more for the numerical solution of these problems.

We address and review some of the results obtained in this research area. Due to the fact, that the integral part produces non-local effects in the evolution process, this is reflected in the numerics by dense matrices which at a first glance slow down the numerical efficiency.

We show first based on a paper by S. and Strauss, how this can be overcome and an efficiency of $O(n \log n)$ can be maintained. This requires a detailed study of the operators and the resulting matrices involved. More recent work by S. and Ye then gives an insight that the interplay between diffusion and nonlocal operators has to be addressed in a more rigorous way.

Current research by S. and Zimmer shows in an interesting numerical study how the issue of preconditioning of some of the PIDE-typical terms should be addressed. At a first glance, the integral operators are - from a functional-analytical point of view - compact operators and therefore no preconditioning should be necessary for the discretized counterparts. However, there are strong theoretical and numerical arguments that the nonlocal term in certain situations does need preconditioning and we show how this can be achieved. We will address also some theoretical issues as well.

**On the concepts of numerical stability in Krylov subspace methods**

**Zdeněk Strakoš** *(Charles University in Prague)*

John von Neumann and Herman H. Goldstine formulated in the paper *Numerical inverting of matrices of high order,* Bull. Amer. Math. Soc., 53 (1947), pp. 1021-1099, which is often considered as the beginning of the field of numerical analysis, the following paragraph concerning the errors in numerical computations:

*"When a problem in pure or in applied mathematics is 'solved' by numerical computation, errors, that is, deviations of the numerical 'solution' obtained from the true, rigorous one, are unavoidable. Such a 'solution' is therefore meaningless, unless there is an estimate*

*of the total error in the above sense.*

*Such estimates have to be obtained by a combination of several different methods, because the errors that are involved are aggregates of several different kinds of contributory, primary errors. These primary errors are so different from each other in their origin and character, that the methods by which they have to be estimated must differ widely from each other. A discussion of the subject may, therefore, advantageously begin with an analysis of the main kinds of primary errors, or rather of the sources from which they spring.*

*This analysis of the sources of errors should be objective and strict inasmuch as completeness is concerned, . . . .”*

In using as well as in analysis of Krylov subspace methods we are faced with different effects of rounding errors. Numerical stability issues (or, more generally, effects of inexactness in computations) that are important in practical applications are investigated using various approaches. Krylov subspaces are based on powering the operator with respect to the given vector that has to be done in a way that balances computational cost and numerical accuracy. Nonlinearity of the methods makes a rigorous and complete analysis very difficult. This leads to using simplifying assumptions that can enable formulation of quantitative results at the price of restricting their applicability to specific classes of problems. Any generalization of the obtained conclusions then requires a careful justification. This contribution will focus on several challenges in that direction.

**Schur complement based block preconditioners for block-structured indefinite linear systems**

**Walter Zulehner** *(Johannes Kepler University Linz)*

Optimality systems of PDE-constrained optimization problems lead—after discretization and linearization—to linear systems of equations in saddle point form with a 2-by-2 block structure associated with the primal and the dual variables (Lagrangian multipliers) of the problem. Often the primal and/or the dual variables have a natural block structure themselves leading altogether to systems with indefinite $N$-by-$N$ block matrices for $N \geq 3$. In this talk we discuss block preconditioners for such matrices based on (a sequence of) Schur complements associated with these block matrices. Following the results in [1], where the case $N = 2$ is considered, we present some generalizations for (small) integers $N \geq 3$.

**References**

[1] Malcolm F. Murphy, Gene H. Golub, and Andrew J. Wathen. A note on preconditioning for indefinite linear systems. *SIAM J. Sci. Comput.*, 21(6):1969–1972, 2000.

## Minisymposium M12

## Singularly perturbed differential equations

Organisers

Niall Madden and Martin Stynes

**Discontinuous Galerkin methods for time-dependent singularly perturbed problems**

**Sebastian Franz** & Gunar Matthies *(TU Dresden)*

We consider a time-dependent problem of the type

$$\begin{aligned} \partial_t u(\mathbf{x},t) + (Lu)(\mathbf{x},t) &= f(\mathbf{x},t) && \text{in } \Omega \times [0,T] \\ u(\mathbf{x},t) &= 0 && \text{on } \partial\Omega \times [0,T] \\ u(\mathbf{x},t) &= u_0(\mathbf{x}) && \text{on } \Omega \times \{0\} \end{aligned}$$

where $L$ is a singularly perturbed spatial operator like

$$\begin{aligned} (Lu)(\mathbf{x},t) &:= -\varepsilon_M \Delta u(\mathbf{x},t) - \mathbf{b}(\mathbf{x},t) \cdot \nabla u(\mathbf{x},t) \\ &\quad + c(\mathbf{x},t)u(\mathbf{x},t), \\ (Lu)(\mathbf{x},t) &:= -\varepsilon_M \Delta u(\mathbf{x},t) - b(\mathbf{x},t)u_x(\mathbf{x},t) \\ &\quad + c(\mathbf{x},t)u(\mathbf{x},t), \\ (Lu)(\mathbf{x},t) &:= -\varepsilon_M \Delta u(\mathbf{x},t) + c(\mathbf{x},t)u(\mathbf{x},t). \end{aligned}$$

Let us apply discontinuous Galerkin methods for the time-discretisation, while the spatial problem is dealt with using some flavour of the finite element method.

We will show an error estimation that separates the temporal error contribution from the spatial error contribution. Numerical simulations support the analytical results for $\Omega \subset \mathbb{R}^2$.

**Grad-div stabilization for the evolutionary Navier-Stokes equations with inf-sup stable infinite elements**

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

The approximation of the time-dependent Navier-Stokes equations using inf-sup stable mixed finite elements in a Galerkin method with grad-div stabilization is studied. The main goal is to prove that adding a grad-div stabilization term to the Galerkin approximations has a stabilizing effect for small viscosity. Both the continuous-in-time and the fully discrete case are considered. Error bounds are obtained that do not

depend on the inverse of the viscosity. These bounds require the solution to have no more than second-order derivatives bounded in $L^2$ at time $t = 0$, since further regularity at $t = 0$ requires the solution to satisfy non-local compatibility conditions difficult to enforce in practical situations. The bounds for the divergence of the velocity as well as for the pressure are optimal. The analysis is based on the use of a specific Stokes projection.

**Numerical solution of singularly perturbed elliptic problems on non-rectangular domains**

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

We are interested in singularly perturbed elliptic problems of the form

$$-\varepsilon\triangle\tilde{u} + (\tilde{a}_1, \tilde{a}_2) \cdot (\tilde{u}_\zeta, \tilde{u}_\eta) + \tilde{b}\tilde{u} = \tilde{f}, \quad (\zeta, \eta) \in \tilde{\Omega},$$

with boundary conditions $\tilde{u} = 0, (\zeta, \eta) \in \partial\tilde{\Omega}$, where

$$\overline{\tilde{\Omega}} := \{(\zeta, \eta) | 0 \le \eta \le 1, \phi(\eta) \le \zeta \le 1 + \phi(\eta); \phi(0) = 0\}.$$

The mapping $F : \tilde{\Omega} \to \Omega := (0, 1)^2$ defined by $x = \zeta - \phi(\eta), y = \eta$ transforms the problem into the following problem for $u(x, y) = \tilde{u}(\zeta, \eta)$ in the unit square $\Omega$:

$$\begin{aligned} -\varepsilon((1 + (\phi')^2)u_{xx} - 2\phi' u_{xy} + u_{yy}) \\ + a_1 u_x + a_2 u_y + bu = f \\ u = 0, (x, y) \in \partial\Omega \\ a_1 = \tilde{a}_1 - \tilde{a}_2\phi' + \varepsilon\phi''; a_2 = \tilde{a}_2(x, y). \end{aligned}$$

The solution of this problem can have exponential boundary layers or parabolic boundary layers depending on the value of $a_1$, which is dependent on both the geometry of the original domain $\tilde{\Omega}$ and $\varepsilon$. We restrict consideration here to the case where $\phi$ is linear; i.e., the domain $\tilde{\Omega}$ is a parallelogram. An analogous problem was studied in [1], where a numerical method was proved to be $\varepsilon$-uniformly convergent under some restrictions. We investigate various ways of treating the mixed derivative term to remove these restrictions.

**References**

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**An efficient and uniformly convergent alternating direction method for solving 2D reaction-diffusion problems with time dependent boundary conditions**

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

In this talk we develop and analyze an efficient uniformly convergent numerical method, of type alternating directions, for solving singularly perturbed problems of the following type:

Find $u(x, y, t) : \bar{\Omega} \times [0, T] \subset \mathcal{R}^3 \to \mathcal{R}$ solution of

$$\begin{cases} \dfrac{\partial u}{\partial t} - \varepsilon^2\Delta u + k(x, y, t)u = f(x, y, t), \text{ in } \Omega \times (0, T], \\ u(x, y, 0) = \varphi(x, y), \text{ in } \Omega, \\ u(x, y, t) = g(x, y, t), \text{ in } \partial\Omega \times [0, T]. \end{cases} \quad (1)$$

where we assume that the reaction term satisfies $k(x, y, t) \ge \beta^2$, $\beta > 0$. We will pay special attention to the singularly perturbed case ($\varepsilon^2 << \beta^2$) where the presence of boundary layers requires the use of fitted space discretization techniques in order to capture successfully the rapid variations of its solutions at these regions.

We will also focus our attention in the order reduction phenomenon, which is typical if alternating direction schemes are chosen to integrate in time and specially severe when time dependent boundary data $g$ are present. Such drawbacks appear when classical evaluations of the boundary conditions are used. We propose a simple modification for these evaluations, easy to implement, and we analyze it in detail, proving that the order reduction is avoided completely. Also, some numerical experiments are shown in order to illustrate the improvements which the method provides.

**Maximum-norm a posteriori estimates for singularly perturbed reaction-diffusion problems on shape-regular and anisotropic meshes**

**Natalia Kopteva** & Alan Demlow *(University of Limerick)*

Our goal is to prove residual-type a posteriori error estimates in the maximum norm for singularly perturbed semilinear reaction-diffusion equations of the form

$$Lu := -\varepsilon^2\triangle u + f(x, u) = 0 \text{ in } \Omega, \quad u = 0 \text{ on } \partial\Omega. \quad (1)$$

Here we assume that $0 < \varepsilon \le 1$, that $f$ is continuous on $\Omega \times R$ and satisfies $f(\cdot, s) \in L_\infty(\Omega)$ for all $s \in R$, and the one-sided Lipschitz condition $f(x, u) - f(x, v) \ge C_f[u - v]$ whenever $u \ge v$. Here $C_f \ge 0$. We additionally assume that $\Omega$ is a, possibly non-Lipschitz, polyhedral domain in $R^n$, $n = 2, 3$. Then there is a solution $u \in H_0^1(\Omega) \cap C(\bar{\Omega})$. (To be more

precise, $u \in W_l^2(\Omega) \subseteq W_q^1 \subset C(\bar{\Omega})$ for some $l > \frac{1}{2}n$ and $q > n$.)

In the first part of the talk, standard finite element approximations are considered on shape-regular meshes [1]. The error constants are independent of the diameters of mesh elements and the small perturbation parameter. In our analysis, we employ sharp bounds on the Green's function of the linearized differential operator. Numerical results are presented that support our theoretical findings.

In the second part of the talk, we shall consider linear finite elements on anisotropic triangulations [2]. The error constants are independent of the diameters and the aspect ratios of mesh elements as well as of the small perturbation parameter. To roughly describe our results, assuming that anisotropic mesh elements are almost non-obtuse, our first estimator reduces to

$$\begin{aligned}\|u-u_h\|_{\infty;\Omega} \leq C\,\ell_h \max_{z\in\mathcal{N}}\Big( & \min\{\varepsilon, H_z\}\,\big\|J_z\big\|_{\infty;\gamma_z} \\ & + \min\{\varepsilon H_z, H_z^2\}\,\|\varepsilon^{-2} f_h^I\|_{\infty;\omega_z}\Big) \\ & + C\,\|f_h - f_h^I\|_{\infty;\Omega}\,, \end{aligned} \tag{2}$$

where $C$ is independent of the diameters and the aspect ratios of elements in the triangulation $\mathcal{T}$, and of $\varepsilon$. Here $\mathcal{N}$ is the set of nodes in $\mathcal{T}$, $J_z$ is the standard jump in the normal derivative of computed solution $u_h$ across an element edge, $\omega_z$ is the patch of elements surrounding any $z \in \mathcal{N}$, $\gamma_z$ is the set of edges in the interior of $\omega_z$, $H_z = \operatorname{diam}(\omega_z)$, $\ell_h = \ln(2 + \varepsilon \underline{h}^{-1})$, and $\underline{h}$ is the minimum height of triangles in $\mathcal{T}$.

**References**


[1] A. Demlow & N. Kopteva, *Maximum-norm a posteriori error estimates for singularly perturbed elliptic reaction-diffusion problems*, 2014, `http://www.staff.ul.ie/natalia/pdf/demlow_kopteva_NM.pdf`.

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### A balanced-norm finite element method for singularly perturbed problems


**Niall Madden**, J.H. Adler & S. MacLachlan *(National University of Ireland Galway)*


We consider the numerical solution, by a Petrov-Galerkin finite-element method, of singularly perturbed reaction-diffusion equations of the form

$$Lu := -\varepsilon^2 \Delta u + bu = f \quad \text{in } \Omega := (0,1)^2,\ u = 0 \ \text{ on } \partial\Omega.$$

Lin and Stynes (SINUM, 2012) observed that the natural energy norm associated with a standard Galerkin approach under-weights the layer component. Their solution to this was to propose a mixed finite element method that gives a solution which is quasioptimal in a so-called "balanced" norm. In the style of a first-order system least squares (FOSLS) method (e.g., Cai et al., SINUM, 1997), we extend the approach of Lin and Stynes by introducing a constraint which simplifies the associated finite-element space and, consequently, the method's analysis and the use of suitable fast solvers [1]. We prove robust convergence in a balanced norm on a piecewise uniform (Shishkin) mesh, and present supporting numerical results.

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### A convection dominated moving pulse


**Eugene O'Riordan** & Jose Luis Gracia *(Dublin City University, Ireland.)*


A singularly perturbed parabolic equation of convection-diffusion type is examined. Initially the solution approximates a concentrated source. This causes an interior layer to form within the domain for all future times. Using a suitable transformation, a layer adapted mesh is constructed to track the movement of the center of the interior layer. A parameter-uniform numerical method, using simple upwinding on this layer-adapted mesh, is constructed and analysed for this problem. Numerical results are presented to illustrate the theoretical error bounds established.

### Sparse grid finite element methods for singularly perturbed problems


**Stephen Russell** & Niall Madden *(National University of Ireland Galway)*


Standard finite element methods (FEMs), such as the Galerkin method with the usual polynomial basis functions are impractical for very large problems, especially in higher dimensions, due to the infamous "curse of dimensionality". Sparse grid methods try to break

this curse by delivering the same order of accuracy as a classical FEM but, through careful choice of basis functions, with far fewer degrees of freedom (ideally, independent of the problem dimension).

For PDEs, sparse grid methods are usually based on the idea of hierarchical basis functions, [3]. An adaptive wavelet based method for singularly perturbed problems has been studied by [4]. Zhou et al. gave an analysis of a simpler, more flexible, "two-scale" sparse grid method, and have successfully applied this to a two-dimensional reaction-diffusion problem on a Shishkin mesh [1]. This approach requires only $\mathcal{O}(N^{3/2})$ degrees of freedom compared to $\mathcal{O}(N^2)$ for the Galerkin FEM, but with no loss of accuracy. In [2] we extend the results of [1] to a multiscale sparse grid method that requires only $\mathcal{O}(N \log N)$ degrees of freedom: that is, we recover the efficiency of the usual sparse grid method, while retaining the essential simplicity of the two-scale approach.

In this talk, we will focus on the design and analysis of the method, and particularly the construction of a special interpolation operator. We conclude with the results of numerical experiments that support the theoretical findings, along with some preliminary findings on how this may be extended to three dimensional problems.

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# Abstracts of Contributed Talks

### Finite Element Methods with Fictitious Domain for Transient Heat Equation: Stability and Convergence Analysis

**Cheherazada Gonzalez Aguayo** *(University of Strathclyde)*

In this work, we are going to consider the stabilized finite element method with fictitious domain for the transient heat problem. We give the full analysis only for the backward difference formula of order one. For that, we prove unconditional stability of $u$ and Lagrange multipliers, and optimal convergence for transient heat problem (in natural norms) when the initial data are chosen as a certain Ritz-type projection. In the case when a standard interpolation of the initial data is applied, an *inverse parabolic Courant-Friedrich-Lewy (CFL)-type* condition must be respected in order to maintain stability for small time steps.

### Numerical Algorithms to Compute the Sine and the Cosine of a Matrix

**Awad Al-Mohy**, Nicholas Higham & Samuel Relton *(King Khalid University)*

The importance of the matrix sine and cosine stems from their role in the solution of second order differential equations $y''(t) + Ay(t) = g(t)$, $y(0) = y_0$, $y'(o) = y_0'$, where $A$ is a square matrix. This equation arises in finite element semidiscretization of the wave equation. We derive new algorithms to evaluate $\sin(A)$ and $\cos(A)$ separately or together employing both Padé approximants of the sine function and new rational approximants to the cosine and sine functions obtained from Padé approximants to the exponential function. By rigorous analysis we prove that the algorithms are backward stable in exact arithmetic and our numerical experiments show that they behave in a forward stable manner in floating point arithmetic and outperform existing algorithms.

### Efficient Iterative Solution Algorithms For Numerical Models of Multiphase Flow

**Ahlam Alrehaili** & Dr. Mark Walkley & Professor Peter Jimack *(University of Leeds)*

In this work we consider efficient numerical methods for the simulation of vascular tumour growth based upon the multiphase model introduced by Hubbard and Byrne [1].

The talk will present a brief overview of the multiphase model, which involves the evolution of four different, but coupled, phases. We will then describe the discretization schemes used to solve the time-dependent system of partial differential equations (PDEs). This involves a finite volume scheme to approximate mass conservation and a conforming finite element scheme to approximate momentum conservation. The latter system is represented as a Stokes-like flow of each phase, with source terms that reflect the phase interactions. It will be demonstrated that the solution of these coupled momentum equations, approximated using Taylor-Hood element in two dimensions, is the most computationally intensive component of the solution algorithm.

The final part of the presentation will provide a detailed description of the structure of these discrete coupled momentum equations, and an assessment of a number of different pre-conditioning strategies for the resulting algebraic system. Results will contrast the different pre-conditioners considered and we will conclude with a discussion of these techniques.

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### Pseudospectra and eigenvalue condition numbers of Fiedler companion matrices

**Javier Pérez Álvaro**, Fernando De Terán & Froilán M. Dopico *(The University of Manchester)*

Computing roots of scalar polynomials as the eigenvalues of Frobenius companion matrices is a classical approach. The introduction of new families of companion matrices allows for the use of other matrices in the root-finding problem. Even though computing the roots of a polynomial and computing the eigenvalues of a companion matrix are mathematically equivalent, these two problems present relevant differences from the numerical point of view. In particular, those regarding conditioning and backward errors. In this talk, we will investigate eigenvalue condition numbers and pseudospectra of Fiedler matrices of a monic polynomial $p(z)$. In particular, we will compare the condition number of a given root of a monic polynomial $p(z)$ with the condition number of this root as an eigenvalue of any Fiedler matrix, and the pseudozero sets of $p(z)$ with the pseudospectra of the associated Fiedler matrices. We will show that if the maximum of the absolute values of the coefficients of $p(z)$ is much larger or much smaller than 1, then the eigenvalues

of Fiedler matrices may be potentially much more ill conditioned than the roots of $p(z)$. By contrast, if the maximum of the absolute values of the coefficients of $p(z)$ is moderate and not close to zero, that is, it is of order $\Theta(1)$, then the eigenvalues of Fiedler matrices and the roots of $p(z)$ are guaranteed to have similar condition numbers, and therefore, from the point of view of eigenvalue condition numbers, in this case all Fiedler companion matrices are good tools for the purpose of computing roots of monic polynomials. We will also study the ratio between eigenvalue condition numbers of Frobenius companion matrices and eigenvalue condition numbers of Fiedler matrices other than the Frobenius ones. We will show that if the absolute value of the coefficients of $p(z)$ are moderate then this ratio is also moderate and, therefore, from the point of view of condition numbers, in this situation any Fiedler matrix can be used for solving the root-finding problem for $p(z)$ with the same reliability as Frobenius companion matrices.

Regarding pseudospectra of Fiedler matrices, first, we will show how to accurately estimate them in a $m \times m$ grid using only $O(nm^2)$ flops compared with the $O(n^3m^2)$ flops needed in SVD methods. Then, we will establish various mathematical relationships between the pseudozero sets of a monic polynomials $p(z)$ and the pseudospectra of the associated Fiedler matrices.

Finally, the effect of balancing Fiedler matrices will also be investigated from the point of view of eigenvalue condition numbers and pseudospectra. We will present numerical evidence that shows the following: if Fiedler matrices are balanced then the roots of $p(z)$ and the eigenvalues of the balanced Fiedler matrices are usually equally conditioned, and that pseudozero sets of $p(z)$ and pseudospectra of Fiedler matrices are usually quite close to each other.

**Finite elements for a class of nonlinear stochastic pdes from phase transition problems**

**Dimitra C. Antonopoulou** *(University of Chester)*

We construct Galerkin numerical schemes with possible discontinuities in time for a class of nonlinear evolutionary pdes with additive noise. These equations appear in phase transitions problems and may involve a positive parameter $\varepsilon$ which stands as a measure for the inner interfacial regions width. Our goal is to establish existence of numerical solution and derive optimal error estimates even for the discontinuous Galerkin case in the presence of noise.
Key words: Finite elements, nonlinear stochastic pdes, dG methods.

**Error analysis of a mixed finite element approximation of Stokes problem with Tresca friction boundary condition**

**Leonardo Baffico** & Taoufik Sassi *(Université de Caen Basse-Normandie)*

We study the error analysis of a mixed finite element approximation of the 2D Stokes problem with Tresca friction boundary condition. This non-linear boundary condition states that the tangential velocity can be different from zero if the absolute value of the shear stress reaches a given threshold function [3]. The variational formulation of this problem corresponds to a variational inequality of the second kind. Since a non-differentiable term is present in this inequality, we use an equivalent three-field mixed variational formulation [1]. The well-posedness of this problem and its finite element approximation is a consequence of two *inf-sup* conditions involving the pressure and the additional Lagrange multiplier associated to the non-linear boundary condition. Using classical tools, we obtain optimal *a priori* error estimates for the *P1 bubble-P1-P1* mixed finite element approximation [2].

Next, in order to complement this theoretical result, we will present numerical results obtained by implementing the mixed approximation using FreeFEM++ [4] and a quadratic programming algorithm [5]. Finally, inspired by [6], we will present an algorithm that splits the three-field variational formulation into two problems: a Stokes problem and a constrained mixed problem involving the fluid velocity and the Lagrange multiplier associated to the boundary condition.

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### A Discontinuous Galerkin Scheme for Modelling Light Scattering in the Human Retina

**Adérito Araújo** & S. Barbeiro & R. Bernardes & F. Caramelo & M. Morgado & L. Pinto & M. Santos & P. Serranho *(University of Coimbra)*

Optical Coherence Tomography, OCT, is a relatively recent imaging technique that allows high resolution imaging of the retina. It relies on certain optical characteristics of light to provide information of the eye fundus, facilitating the diagnosis of certain eye pathologies. In this talk we will discuss the mathematical model that describes the electromagnetic wave's propagation through the eye's structures in order to create a virtual OCT scan. Our model is based on time-dependent Maxwell's equations. We use the discontinuous Galerkin method for the integration in space and a low-storage Runge-Kutta method for the integration in time. To validate the proposed methodology, we compare the results with Mie's solution to Maxwell's equations, which only describes the scattering patterns for homogeneous spheres. This is a mandatory step before further elaborating the numerical scheme towards the propagation of electromagnetic waves through the human retina. We also present an application of our methodology to the assessment of cell level alterations responsible for the OCT data in Diabetic Macular Edema.

### A contribution to the theory of the sweeping preconditioner for the Helmholtz equation

**Elizabeth Arter** & Euan Spence & Ivan Graham *(University of Bath)*

In 2011 Engquist and Ying introduced the sweeping preconditioner for the Helmholtz equation discretised on tensor-product grids by low-order finite element or finite difference methods. This method starts from the block Thomas algorithm, and shows that certain Schur complements that appear are low rank. Approximating these low-rank blocks then leads to an effective preconditioner. The approximation is usually made on the discretization of the damped Helmholtz equation and then used to precondition the Helmholtz equation, and this talk provides a contribution to the theoretical understanding of the method.

### A priori finite element error analysis for problems with low regular solutions

**Sílvia Barbeiro** *(CMUC, University of Coimbra)*

We consider the numerical solution with finite element methods of elliptic boundary value problems with both inhomogeneous Dirichlet and Neumann boundary conditions. The focus of this talk is to derive $L^2$ error estimates without restrictive regularity assumptions on the solutions of the original and adjoint problems. We analyze in particular the effect of the choice of the discrete Dirichlet data on the estimates. To illustrate the theoretical results, some numerical examples will be presented.

### Asynchronous multi-time-step domain decomposition method for evolution problems

**Michal Beneš** *(Czech Technical University in Prague)*

Evolution of time dependent physical quantities such as current, heat etc., in composite materials are modelled by initial boundary value problems for parabolic PDEs. These physical quantities follow different evolution patterns in different parts of the computational domain depending on the material properties, size of constituent material subdomains, coupling scheme, etc. Therefore, the stability and accuracy requirements of a numerical integration scheme may necessitate domain dependent time discretization. Parabolic problems are usually solved by discretizing spatially using finite elements and then integrating over time using discrete solvers. We propose an asynchronous multi-domain time integration scheme for parabolic problems. For efficient parallel computing of large problems, we present the dual decomposition method with local Lagrange multipliers to ensure the continuity of the primary unknowns at the interface between subdomains. The proposed method enables us to use domain dependent Rothe method on different parts of a computational domain and thus provide an efficient and robust approach to solving large scale problems.

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### Linear barycentric rational interpolation with guaranteed degree of precision

**Jean–Paul Berrut** *(University of Fribourg, Switzerland)*

Changing the weights in the barycentric formula for polynomial interpolation to other non–negative values yields a rational interpolant. In a 1988 paper, I have suggested to order the nodes $x_j$ according to $x_0 < x_1 < x_2 < \ldots < x_n$ and to take the weights all equal, but with alternating signs. This guarantees that the corresponding interpolant $r_n$ does not have any pole in $[x_0, x_n]$. The convergence of $r_n$ toward an interpolated function $f$ is a slow $\mathcal{O}(h)$, where

$h := \max_{j=0,\dots n-1}(x_{j+1} - x_j)$. Motivated by rational trigonometric interpolation, a second interpolant, in which the first and last weight are halved, was also presented; it has been proved by Floater and Hormann to converge as $\mathcal{O}(h^2)$ for equispaced nodes (the convergence for general sets of nodes is an open question). Both interpolants are exceptionally stable (Bos et al. have shown that the Lebesgue constant of the first grows logarithmically) and nothing like a Runge phenomenon arises.

The Floater–Hormann weights are one way of increasing the order of convergence beyond the value two. In this talk we extend our original approach: we set again $n + 1 - d$ weights equal to $\pm 1$ and choose the remaining $d$ ones in such a way that the resulting $r_{n,d}$ interpolates exactly the first monomials $x^k$, $k = 1, \dots, d$ (constants are interpolated exactly by all barycentric rational interpolants). $r_{n,d}$ is shown experimentally to have convergence order $d$. Since its weights do not depend on the interpolated function, the corresponding approximation operator remains linear.

**An adaptive algorithm for PDE problems with random data**

**Alex Bespalov** & David Silvester *(University of Birmingham)*

In this talk, we present an adaptive algorithm for computing stochastic Galerkin finite element approximations for a class of elliptic PDE problems with random data. Specifically, we assume that the underlying differential operator has affine dependence on a large, possibly infinite, number of random parameters. Stochastic Galerkin approximations are then sought in the tensor product space $X \otimes \mathcal{P}$, where $X$ is a finite element space associated with a physical domain and $\mathcal{P}$ is a set of multivariate polynomials over a finite-dimensional manifold in the (stochastic) parameter space.

Our adaptive strategy is based on computing two error estimators (the spatial estimator and the stochastic one) that reflect two distinct sources of discretisation error and, at the same time, provide effective estimates of the error reduction for the corresponding enhanced approximations. In particular, our algorithm adaptively 'builds' a polynomial space over a low-dimensional manifold in the infinitely-dimensional parameter space such that the discretisation error (in the energy norm) is reduced most efficiently.

Convergence of the adaptive algorithm is demonstrated numerically.

**Computing spectral properties of boundary integral operators in three dimensions with BEM++**

**Timo Betcke** *(University College London)*

Boundary element methods have become a widely used tool in engineering to solve a range of partial differential equation problems in homogeneous media. Yet, many of the spectral properties of boundary integral operators are only little investigated. Even the question of normality is not yet fully understood for scattering problems on domains other than the unit sphere.

In this talk we give an overview of some existing spectral results and their applications and demonstrate numerically spectral properties of boundary integral operators for three dimensional electrostatic, acoustic and electromagnetic problems.

The numerical examples are computed using the open-source boundary element package BEM++ developed at UCL and we will give short demonstrations that show how integral operators for complicated problems can be setup and investigated in just a few lines of code in BEM++.

**Domain Decomposition Methods for the Neutron Transport Equation**

**Jack Blake** & Ivan Graham & Alastair Spence *(University of Bath)*

We consider solving the neutron transport equation using domain decomposition iterative methods. This equation governs the behaviour of neutrons within a reactor and describes the behaviour of the *neutron flux* denoted $\psi(\mathbf{r}, \Omega)$, where $\mathbf{r} \in V \subset \mathbb{R}^3$ is the neutron's location in a 3D coordinate system ($V$ is a bounded spatial domain) and $\Omega \in \mathbb{S}^2$ (the unit sphere in $\mathbb{R}^3$) is its direction of travel. The quantity $\psi(\mathbf{r}, \Omega)$ is then the density of neutrons passing through a unit space at $\mathbf{r}$ in direction $\Omega$ per unit time. The transport equation describes the behaviour of the neutron flux based upon likelihoods of various neutron interactions (or collisions) occurring, and based on the characteristics of a *neutron source*. When modelling a nuclear reactor, it is generally specified that neutrons can undergo three types of interaction: they can be *scattered*, they can be *captured*, or they can cause a *fission* event, though in this talk we will not consider fission interactions. The *absorption cross-section*, denoted $\sigma_A(\mathbf{r})$, is the likelihood of a capture interaction occurring and the neutron ceasing travelling. We denote by $\sigma_S(\mathbf{r})$ the *scattering cross-section*, which is the likelihood that a neutron is scattered and ends up travelling in a new direction. Lastly we denote by $\sigma_T(\mathbf{r})$ the *total*

*cross-section*, which is the likelihood of any collision occurring and satisfies $\sigma_T(\mathbf{r}) = \sigma_S(\mathbf{r}) + \sigma_A(\mathbf{r})$. The *neutron source* term will be denoted by $Q(\mathbf{r})$ and is a non-fission source term, isotropic in angle, of neutrons from position $\mathbf{r}$. Under this notation the transport equation has the following form:

$$\Omega \cdot \nabla\psi(\mathbf{r},\Omega) + \sigma_T(\mathbf{r})\psi(\mathbf{r},\Omega) = \frac{\sigma_S(\mathbf{r})}{4\pi}\int_{\mathbb{S}^2} \psi(\mathbf{r},\Omega)\,\mathrm{d}\Omega + Q(\mathbf{r}),\ \mathbf{r}\in V,\ \ \Omega\in\mathbb{S}^2, \quad (1)$$

subject to suitable boundary conditions on the boundary of $V$.

Although highly non-symmetric, this equation has an equivalent symmetric integral equation formulation. Using this formulation it can be proved that if $\sigma_S$ is smaller than $\sigma_T$ everywhere, then a simple fixed-point iteration involving repeated solutions of (1) converges. If there are subdomains in which $\sigma_S$ is close to $\sigma_T$ then the fixed-point iteration typically converges slowly, but if a certain correction step is included then a fast rate of convergence can be recovered. This motivates the use of domain decomposition iterative methods in which the choice of subdomains is dictated by these material properties.

We will present domain decomposition algorithms whereby in different subdomains the choice of iterative method is driven by the material properties. We will conclude with some numerical results showing how this approach can help find a beneficial compromise between quickly converging methods and computationally cheap methods.

### A promising DPG method for the (stationary) transport equation

**Dirk Broersen** *(University of Amsterdam)*, Wolfgang Dahmen *(RWTH, Aachen)*, Rob Stevenson *(University of Amsterdam)*

A Discontinuous Galerkin finite element method will be presented for the stationary transport problem. Here, an optimal test space is introduced to get the best approximation to the solution from the trial space. To arrive at an implementable method, the truly optimal test space often has to be replaced by its projection onto a finite dimensional *test search space*. However, if the underlying test space is a *broken* space, one can determine the optimal test space analytically and locally, thereby reducing computational costs. In the case of constant convection, these functions are typically piecewise polynomials.

In the case of a non-constant convection term, determining the exact optimal test space gets more complicated. Replacing the convection term by a piecewise constant approximation, knowing the local optimal test functions from the case of constant convection then allows one to construct a test search space for which stability can be proved.

Our findings will be illustrated with several numerical examples.

### Populations of Models for Stochastic Differential Equations

**Pamela M. Burrage** & Kevin Burrage *(Queensland University of Technology)*

The Populations of Models technique is a new modelling approach in which the inherent variability in dynamical processes can be captured by generating sets of parameter values for a given mathematical model that have been successfully calibrated against experimental data and observations. The construction of the population is via Latin Hypercube or Orthogonal Sampling. In this presentation we show how these ideas can be applied to building Populations of Models based on a stochastic mathematical model. We illustrate these ideas by considering several stochastic differential equation models and give some probabilistic interpretation of forward prediction. We also provide estimates for the coverage of parameter space under both Latin Hypercube and Orthogonal Sampling. In addition, we investigate the combination of Latin Hypercube Sampling with Polynomial Chaos expansions for solving a stochastic differential equation.

**Note:** Aspects of this work involving coverage of parameter space under different sampling regimes is joint work additionally with D. Donovan, B. Thompson and T. McCourt.

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### On a Sub-Stiefel Procrustes Problem Arising in Computer Vision

**João R. Cardoso** & Krystyna Zięţak *(Coimbra Institute of Engineering)*

A sub-Stiefel matrix is a matrix that results from deleting simultaneously the last row and the last column of an orthogonal matrix. In this talk we consider a Procrustes problem on the set of sub-Stiefel matrices of order $n$. For $n = 2$ this problem has arisen in computer vision to solve the surface unfolding problem considered in [2]. In a few words, this problem consists of reconstructing smooth, flexible and isometrically embedded flat surfaces, such as a sheet of paper or a flag waving in the wind, from a set of projected observations such as camera images. An iterative algorithm for computing the solution of the sub-Stiefel Procrustes problem for an arbitrary $n$ is proposed and some numerical experiments are carried out to illustrate its performance. For these purposes we investigate the properties of sub-Stiefel matrices. Full details can be found in [1].

Joint work with Krystyna Zięţak *(Wrocław School of Information Technology)*. The speaker acknowledges the funding from Institute of Systems and Robotics–Coimbra, Portugal.

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### A Fractional-Order Variation Based Image Co-Registration Model

**Ke Chen** & Jianping Zhang *(CMIT, University of Liverpool)*

Fractional order derivatives are increasingly used to model various problems in Numerical Analysis. In this talk, a total fractional-order variation regularizer is used to model image inverse problems, the image co-registration in particular, which constructs an index function mapping two given image functions so that features are aligned to each other.

Many deformable registration techniques may lead to unsteady deformation (e.g. not one to one) if the dissimilarity between the reference and template images is too large. A fractional-order derivatives based regularizer (using nonlocal information) offers advantages over competing regularizers with integer order derivatives (first order gradients and second order Laplacians), and is potentially useful for accurate deformation registration. We discuss the theories, numerical algorithms and applications, with our numerical implementation combining the semi-implicit update and conjugate gradients (CG) solution to solve the underlying nonlinear systems. Some brief discussion on image denoising models is also presented. Numerical experiments, including applications to biomedical imaging, will show substantial improvements in accuracy and robustness over the conventional image registration approaches.

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### On efficient numerical methods for unidirectional models of nonlinear-optics

**Raimondas Čiegis** & Sh. Amiranashvili & M. Radziunas *(Vilnius Gediminas Technical University, Lithuania)*

We present and analyze different splitting algorithms for numerical solution of both the generalized nonlinear Schrödinger equation (GNSE)

$$i\partial_z\psi + \sum_{m=2}^{M} \frac{\beta_m}{m!}(i\partial_\tau)^m\psi + \frac{n_2}{c}(\omega_0 + i\partial_\tau)|\psi|^2\psi = 0 \quad (2)$$

and the forward Maxwell equation (FME)

$$(\partial_z + \widehat{\beta})E + \frac{\xi^{(3)}}{2c}\widehat{n}^{-1}\partial_t(E^3) = 0 \qquad (3)$$

describing propagation of wave packets with special emphasis on applications to nonlinear fiber-optics. Here $E(z,t)$ defines a polarized wave, $\tau = t - z/V$ is so-called retarded time, $\psi(z,\tau)$ defines the complex envelope

$$E)z,t) = \frac{1}{2}\psi(z,\tau)e^{i(\beta_0 z - \omega_0 t)} + c.c, \quad \tau = \beta_1 z.$$

While numerical properties of discrete algorithms for GNSE are quite well investigated, the numerical methods for FME are much less known. Our main goal is to select appropriate numerical solvers for both problems and to compare their efficiency when they are used to solve the GNSE and FME.

We investigate the optimality of the following alternatives:

- Finite difference method versus spectral method;
- Full approximation algorithms versus splitting algorithms.

We split the diffraction and nonlinear interaction processes by using the symmetrical Strang splitting approach. After splitting, the nonlinear interaction in FME (2) is defined by the nonlinear Burgers type equation

$$\partial_z \widetilde{E} + \frac{\xi^{(3)}}{2c}\widehat{n}^{-1}\partial_t(\widetilde{E}^3) = 0 \tag{4}$$

and special monotone or TVD approximations are required to approximate the weak solution of this problem.
Finally, FME can be solved in a moving frame by setting $E(z,t) = F(z,\tau)$, where $\tau = t - z/V$ is related to some typical velocity $V$, e.g., the group velocity of the main pulse. Then we get the model

$$(\partial_z + \widehat{\beta}V^{-1}\partial_\tau)F + \frac{4n_2}{3c}\partial_t(F^3) = 0. \tag{5}$$

### Long-time, large-scale simulation of mantle convection

**Samuel Cox**, Andrea Cangiani & Emmanuil Georgoulis *(University of Leicester)*

Whole-earth mantle convection simulation requires large numbers of degrees of freedom to capture the lengthscales necessary for accurate solution, given the nonlinearity of the mechanisms responsible. Adaptivity is a crucial tool in attempts to model with resolutions approaching 10km, while highly parallelised code is required to solve the system in a reasonable time, particularly when modelling long time periods. This talk will discuss some ongoing work to implement this technique for the Boussinesq model, using *a posteriori* error estimators for the underlying Stokes and convection-diffusion equations in a parallelised FEM scheme, with the aim of modelling the full mantle over 100 million years.

### A finite volume scheme for complex diffusion models in image processing

**E. Cuesta** *(University of Valladolid, Spain)* & A. Durán *(University of Valladolid, Spain)* & A. Araujo *(University of Coimbra, Portugal)* S. Barbeiro *(University of Coimbra, Portugal)*

In this talk a finite volume method for a complex PDE based diffusion model of the form

$$\begin{cases} u_t(\mathbf{x},t) &= \operatorname{div}(D(\mathbf{x},t,u)\nabla u(\mathbf{x},t)), \\ & \quad (\mathbf{x},t) \in \Omega \times (0,T], \\ u(\mathbf{x},0) &= u_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \\ \dfrac{\partial u}{\partial n}(\mathbf{x},t) &= 0, \quad (\mathbf{x},t) \in \partial\Omega \times (0,T], \end{cases} \tag{1}$$

where $\Omega \subset \mathbb{R}^2$ with boundary $\partial\Omega$, and $n$ denotes the outer normal, is presented. In (1) $u : \Omega \times (0,T] \to \mathbb{C}$, is complex–valued due to the fact that diffusion in (1) is governed by a complex term $D(\mathbf{x},t,u)$. The IBVP (1) has been proposed for image processing in the framework of PDEs in [4]. This is based on considering the restored image as a complex function $u$ evolving in time according to a multi–scale process [1], where the restoration is handled by means of the complex–valued diffusion term $D$ from the noisy original image $u_0$ in a nonlinear way. The smoothing–enhancing process, typical of the nonlinear real models for denoising [6] is here shared by the real and imaginary parts of the image $u$. The talk will be focused on the description of the finite volume method applied to discretize (1), and its applications to image processing. Comparison with other numerical approaches [2], and with finite volume schemes for real models [3, 5] will be emphasized.

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### Numerical analysis of cordial Volterra integral equations

**Teresa Diogo** *(Instituto Superior Técnico/CEMAT-Lisbon University)*

We consider the so-called cordial Volterra integral equations

$$\mu u(t) = (V_\varphi u)(t) + f(t), \tag{1}$$

where $\varphi \in C^1[0,T]$ is the core of the cordial operator

$$(V_\varphi u)(t) = \int_0^t \frac{1}{t}\,\varphi(s/t)y(s)ds. \tag{2}$$

The operator $V_\phi$ is noncompact in $C[0,T]$ and difficulties arise when proving convergence of numerical methods. In the case of the standard spline collocation method, a certain applicability condition becomes crucial in the convergence analysis ([1], [2]). Although an analytical study of the applicability of the method becomes complicated in the case of cubic and higher order splines, a numerical check is rather simple and this is illustrated by some numerical examples.

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## Study of flows in heterogeneous porous media

N. Djedaidi & **F.Z. Nouri** *(Badji-Mokhtar University, Algeria)*

In this work, we consider flows in hydro-systems including soil and geologically complex and heterogeneous aquifers. Several authors have studied this case, for example, the multiphase problem in multilayer coastal aquifers, was considered among others by Huyakorn et al [3.] A comparison between the multiphase problem and the monophase one (water) with two components (water and salt) was investigated by Hinkelmann et al [4]. It should be noted that at low concentrations, methane is soluble in water, where it builds no new phase but a second component. This requires the study of two phases (fresh water, salted water) with two components (water and methane). Here we consider the case of a coastal aquifer subject to saline intrusion, taking into account the fluid immiscibility. We present a study of the existence and uniqueness of the solution of the coupled model, using results obtained by Gasmi and Al [1] and [2].

### Mathematical model

Let $\Omega$ be an open bounded connected domain of $\mathbb{R}^2$ ($d = 2$ *or* 3), describing the porous medium (aquifer), with Lipschitz boundary $\Gamma$. We consider incompressible flows with constant dynamic viscosities and where the effect of gravity is neglected. The system of equations for the flow of two immiscible fluid phases in porous media is given by

$$\phi\frac{\partial(\rho_\alpha S_\alpha)}{\partial t} + \nabla.(\rho_\alpha v_\alpha) = \rho_\alpha q_\alpha \quad \text{with } v_\alpha$$
$$= -K\frac{k_{r\alpha}(S_\alpha)}{\mu_\alpha}\nabla p_\alpha \quad \text{and } \alpha = f, s$$

where $\varphi$ and $K$ are the porosity and the absolute permeability of the porous medium; $\alpha = f$ denotes the wetting phase, $\alpha = s$ indicates the non-wetting phase. The parameters $S_i$, $v_{i,}$, $p_i$, $k_i$, $\mu_\alpha$ and $q_\alpha$ are the saturation, the velocity, the pressure, the relative permeability, the viscosity and the dynamic source of the term of the $\alpha$-phase, respectively.The main difficulty of this system is to prove the existence and uniqueness of the solution. Therefore by using some physical criteria of the medium and equation (1), we derive a simplified model.

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## GPU accelerated algorithms for computing matrix function vector products

**Megan Farquhar** & Timothy Moroney, Qianqian Yang, Ian Turner *(Queensland University of Technology)*

The efficient computation of matrix function vector products has become an important area of research in recent times, driven in particular by two important applications: the numerical solution of fractional partial differential equations and the integration of large systems of ordinary differential equations. In this work we consider a problem that combines these two applications, in the form of a numerical solution algorithm for fractional reaction diffusion equations that after spatial discretisation, is advanced using the exponential Euler method. We focus on the efficient implementation of the algorithm on Graphics Processing Units

(GPU), as we wish to make use of the increased computational power available with this hardware. We compute the matrix function vector products using the contour integration method in [1]. Multiple levels of preconditioning are applied to reduce the GPU memory footprint and to further accelerate convergence. We also derive an error bound for the convergence of the contour integral method that allows us to pre-determine the appropriate number of quadrature points. Results are presented that demonstrate the effectiveness of the method for large two-dimensional problems, showing a speed-up of more than an order of magnitude compared to a CPU-only implementation.

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**Mind the duality gap: safer rules for the Lasso**

**Olivier Fercoq** & Alexandre Gramfort & Joseph Salmon *(Telecom ParisTech)*

Screening rules allow early discard of irrelevant variables from the optimization in Lasso problems (*i.e.,* $\ell_1$-regularised least squares), or its derivatives, making solvers faster.

In this talk, we propose new versions of the so-called safe rules for the Lasso. Based on duality gap considerations, our new rules create safe test regions whose diameters converge to zero, provided that one relies on a converging solver. This property helps screening out more variables, for a wider range of regularisation parameter values. In addition to faster convergence, we prove that we correctly identify the active sets (supports) of the solutions in finite time.

While our proposed strategy can cope with any solver, its performance is demonstrated using a coordinate descent algorithm particularly adapted to machine learning use cases. Significant computing time reductions are obtained with respect to previous safe rules.

**Augmented Lagrangians, non-negative QP and extensions**

**Roger Fletcher** *(University of Dundee)*

Augmented Lagrangians are not commonly used to solve quadratic programming (QP) problems with inequality constraints due to second derivative discontinuities in both the inner and outer iterations. For non-negative QP (that is the only constraints on the variables are $x \geq 0$) a transformation of variables is described that removes these discontinuities from the inner iteration which can then be solved simply as a system of linear equations. The outer iteration objective function retains second derivative discontinuities but under mild assumptions is strictly convex, and can, for example, be minimized quickly and efficiently by Newton's method with a suitable line search. The method avoids the combinatorial difficulties associated with active set methods and convergence is guaranteed. Extension of these ideas to include $m$ equality constraints on the variables is described. These are particularly effective in the case $m = 1$. Inverse problems provide a rich source of these problem types, and numerical examples of these are described.

**Some numerical solutions of Maxwell equations**

**Liping Gao** *(China University of Petroleum)*

This talk is concerned with a new finite difference method of the 2D Maxwell's equations in time domain. This method is based on the central difference formulas for spatial derivatives over the Yee's staggered points and approximation of the field functions of time by Taylor's polynomials of high degrees. It is shown that the new method is second order accurate in space and any order accurate in time. By Fourier method it is proved that this method is stable when a criterion ( which is weaker than the CFL condition) is satisfied. Numerical experiments to compute the errors, convergence rates, to test energy conservation, and to simulate a wave propagation generated by a point source in a waveguide for the are carried out. Computational results confirm validity of the method.

**Hodge decomposition for two-dimensional time harmonic Maxwell's equations: impedance boundary condition**

**J. Gedicke** & S.C. Brenner & L.-Y. Sung *(Louisiana State University)*

We extend the Hodge decomposition approach for the cavity problem of two-dimensional time harmonic Maxwell's equations to include the impedance boundary condition, with anisotropic electric permittivity and sign changing magnetic permeability. We derive error estimates for a $P_1$ finite element method based on the Hodge decomposition approach and develop a residual type *a posteriori* error estimator. We show that adaptive mesh refinement leads empirically to smaller errors than uniform mesh refinement for numerical experiments that involve metamaterials and electromagnetic cloaking. The well-posedness of the cavity problem when both electric permittivity and

magnetic permeability can change sign is also discussed and verified for the numerical approximation of a flat lens experiment.

### HNA BEM for Multiple Scattering Problems

**A. Gibbs**, S.N. Chandler-Wilde, S. Langdon, A. Moiola *(University of Reading)*

Standard numerical schemes for scattering problems have a computational cost that grows at least in direct proportion to the frequency of the incident wave. For many problems of scattering by single obstacles, it has been shown that a careful choice of approximation space, utilising knowledge of high frequency asymptotics, can lead to numerical schemes whose computational cost is independent of frequency. Here, we extend these ideas to multiple scattering configurations, focusing in particular on the case of two scatterers, with one much larger than the other.

### Efficient merging of multiple segments of Bézier curves

**Przemysław Gospodarczyk**, Paweł Woźny & Stanisław Lewanowicz *(University of Wrocław)*

We present a novel approach to the *merging problem of segments of a composite Bézier curve* under the *parametric continuity conditions*, with respect to the *least squares norm*. More precisely, we consider the following *approximation problem*.

Let $0 = t_0 < t_1 < \ldots < t_s = 1$ be a partition of the interval $[0, 1]$. Let there be given a *composite Bézier curve* $P(t)$ ($t \in [0, 1]$) which in the interval $[t_{i-1}, t_i]$ ($i = 1, 2, \ldots, s$) reduces to a *Bézier curve* $P^i(t)$ of degree $n_i$, i.e.,

$$P(t) = P^i(t) := \sum_{j=0}^{n_i} p_j^i \, B_j^{n_i}\left(\frac{t - t_{i-1}}{t_i - t_{i-1}}\right) \quad (t_{i-1} \le t \le t_i),$$

where $p_j^i \in \mathbb{R}^d$ are called *control points*, and

$$B_j^n(t) := \binom{n}{j} t^j (1-t)^{n-j} \qquad (0 \le j \le n)$$

are *Bernstein basis polynomials* of degree $n$. Find a degree $m$ ($\ge \max_i n_i$) Bézier curve

$$R(t) := \sum_{j=0}^{m} r_j \, B_j^m(t) \qquad (0 \le t \le 1)$$

such that the error

$$\int_0^1 \|P(t) - R(t)\|^2 \, \mathrm{d}t$$

is minimized in the space $\Pi_m^d$ of parametric polynomials in $\mathbb{R}^d$ of degree at most $m$ under the following parametric continuity conditions:

$$R^{(i)}(0) = P^{(i)}(0) \qquad (i = 0, 1, \ldots, k-1),$$
$$R^{(j)}(1) = P^{(j)}(1) \qquad (j = 0, 1, \ldots, l-1),$$

where $k \le n_1 + 1$, $l \le n_s + 1$, and $k + l \le m$. Here $\|\cdot\|$ is the Euclidean vector norm.

Thanks to the fast schemes of evaluation of certain connections involving Bernstein and *dual Bernstein polynomials*, the complexity of our algorithm is $O(sm^2)$, which is significantly less than the complexity of other known methods (see, e.g., [1] and the extensive list of references given there). Moreover, since our approach avoids solving a system of normal equations, matrix inversion is not required. We give some illustrative examples to demonstrate the effectiveness of our algorithm. See the preprint [2].

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### Domain decomposition for high-frequency Helmholtz problems using absorption

**Ivan Graham** & Euan Spence & Eero Vainikko *(University of Bath)*

We give new results on domain decomposition preconditioners for GMRES when used to solve low order finite element approximations of the Helmholtz equation $-\Delta u - (k^2 + i\varepsilon_M)u = f$, with absorption parameter $\varepsilon_M \ge 0$.

Multigrid approximations of this equation with $\varepsilon_M > 0$ are commonly used as preconditioners for the pure Helmholtz case ($\varepsilon_M = 0$). However a rigorous theory for such (so-called "shifted Laplace") preconditioners, either for the pure Helmholtz equation or even the damped equation is still missing.

We present a new theory for the damped equation which provides rates of convergence for (left- or right-) preconditioned GMRES, via estimates of the norm and field of values of the preconditioned matrix.

Numerical experiments (in 2D) illustrate the theory and also give insight into how domain decomposition approximations of the damped problem perform as

preconditioners for the pure Helmholtz case. For this case a scalable solver with empirical complexity about $\mathcal{O}(n^{4/3})$ is presented.

### A Numerical Result for a Drug Response Mathematical Model

**A. Hadji** & M.L. Hadji *(Badji-Mokhtar University, Algeria)*

In this work we propose a numerical scheme to solve a problem, modeling the drug response. Pharmacogenomics uses a person's genes to explain the difference between how one person responds to a drug compared to another. The mathematical modeling takes this field one step further by also including information about how the body processes a drug and how the drug acts in the body, see for example [1] and [2].

Here we first present the mathematical model, namely a partial differential equation of reaction diffusion type. Then we propose our numerical scheme, that is based on finite differences and a discontinuous Galerkin finite element method [3], for time and space discretisations, respectively. By numerical experimentations, we prove and illustrate the direct benefit and potentiality of our proposed scheme by the performance and the competitive results, yielding information on pharmacological targets.

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### Wedge-shaped generalization of Jacobi matrices

**Iveta Hnětynková** & Martin Plešinger *(Institute of Computer Science, Czech Academy of Sciences and Charles University in Prague; Technical University of Liberec)*

Jacobi matrices, i.e. symmetric tridiagonal matrices with positive subdiagonal entries, represent thoroughly studied objects appearing in many areas of mathematics. They are closely connected to the Lanczos tridiagonalization, the Golub-Kahan bidiagonalization, the Gauss quadrature, moment problems, orthogonal polynomials, etc.; see [2]. Well known spectral properties of Jacobi matrices include simple eigenvalues, the strict interlacing property of eigenvalues, nonzero first and last entries of eigenvectors, etc.; see [3, Chapter 7, pp. 119–150].

The paper [1] introduced the so called $\rho$-wedge-shaped matrices that can be seen as a generalization of Jacobi matrices. The definition was motivated by the structure of matrices obtained as outputs of the band (or block) generalization of the Golub-Kahan bidiagonalization and the band (or block) Lanczos algorithm with deflations. Here the starting vector $b \in \mathbb{R}^n$ is replaced by a matrix $B \in \mathbb{R}^{n\times p}$.

In this presentation, we study the $\rho$-wedge-shaped matrices. We concentrate especially on analysis of their spectral properties and their relationship to the band (or block) algorithms mentioned above.

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### Multilevel Monte Carlo Methods in Atmospheric Dispersion Modelling

**Grigoris Katsiolides** *(University of Bath)*

Monte Carlo methods are used for numerical approximations in a wide area of fields such as mathematics, physics, biology and finance. The Multilevel Monte Carlo(MLMC) method has shown great potential for reducing the computational complexity of the algorithm from $O(\epsilon^{-3})$ to $O(\epsilon^{-2})$, where epsilon is the total error. We present how the MLMC method can be applied in Atmospheric Dispersion modelling which is used to predict the spread of atmospheric pollutants (such as volcanic ash) in operational forecasting and emergency response and thus requires the fast solution of a stochastic differential equation (SDE). We examine how the efficiency of the method is affected by using various time-step methods and by adding suitable boundary conditions.

### Numerical solution for fourth-order two-point boundary value problems based on exponential

**sextic spline**

**Pooja Khandelwal** & Arshad Khan *(Jamia Millia Islamia, India)*

In this paper, we develop a generalized scheme based on exponential sextic spline function for the numerical solution of fourth-order two-point boundary value problems occurring in a plate deflection theory. Spline relations and error estimates are given. Direct methods of order two, four and six have been obtained. Convergence analysis of methods have been discussed. The proposed method is tested on several linear and nonlinear problems. Comparisons are made to confirm the reliability and accuracy of the proposed technique.

**Numerical solution of time-space fractional bio-heat equation using cubic B-spline method**

**Sushil Kumar** *(S.V. National Institute of Technology Surat-India)*

In the present paper a numerical method based on cubic B-splines is used to solve a time-space fraction bio heat equation in biological tissue. The fractional time derivative $\alpha \in (0, 1]$ is considered of Caputo form and is approximated using quadrature formula, while space derivative $\beta \in (1, 2]$ is approximated with cubic B-splines. Temperature profiles in tissue are obtained for different values of $\alpha$ and $\beta$ to study the effect of anomalous diffusion.

**Using matrix scaling to identify block structure**

**Philip Knight** & Iain Duff, Sandrine Mouysset, Daniel Ruiz, Bora Ucar. *(University of Strathclyde)*

We can apply a two-sided diagonal scaling to a non-negative matrix to render it into doubly stochastic form if and only if the matrix is fully indecomposable. The scaling often reveals key structural properties of the matrix as the effects of element size and connectivity are balanced. Exploiting key spectral properties of doubly stochastic matrices, we will show how to use the scaling to reveal hidden block structure in matrices without any prior knowledge of the number and size of the blocks. In particular, the structure of the basis of the principal singular vectors of the scaled matrix allows us to perform a multi-way partition of the rows and columns of the matrix in the spirit of the Fiedler vector. The application of a Canny filter to one or more singular vectors allows us to detect the number of clusters automatically.

**Application of the SQP Method for Finding Error Trajectories of a Dynamical System**

**Jan Kuřátko** & Stefan Ratschan *(Charles University in Prague; The Czech Academy of Sciences)*

We study the problem of finding a trajectory of a given dynamical system so that it originates in a given set of initial states and reaches a given set of unsafe states. We call a trajectory from an initial state to an unsafe state an *error trajectory* of a system. This problem of computing a trajectory resembles the classical boundary value problem (BVP). However, it differs due to the fact that we do not consider any time horizon and we seek a trajectory of arbitrary length.

We formulate the problem of finding error trajectories as a continuous optimization problem and apply the *Sequential Quadratic Programming* (SQP) method. We consider different variants of the formulation of the optimization problem, investigate their properties and compare them. We introduce regularization and adaptive techniques that we use during computation, present numerical results and discuss the structure and sparsity of the resulting Hessian of the Lagrangian.

**Overcoming the sign conflict problem in H (curl)-conforming hexahedral *hp*-finite elements**

**R M Kynch** & P D Ledger *(Swansea University)*

In practical applications of problems in electromagnetism it is necessary to deal with complex geometrical configurations. Although unstructured tetrahedral meshes are capable of describing complex geometrical configurations they are less computationally efficient when it comes to filling large free space regions. Hexahedral elements, on the other hand, offer computational efficiency for filling free space and tend to lead to greater accuracy for the same number of unknowns. Thus combinations of hybrid meshes of tetrahedra, prisms and pyramids and hexahedra are useful in certain applications.

A common issue associated with hierarchic *hp*-finite element shape functions is the sign conflict issue, which arises due to contrasting edge (and face) parameterisations. This issue is particularly evident in H(curl)-conforming finite elements required for Maxwell's equations. In two–dimensional situations this does not present a significant challenge. However, in three–dimensions the presence of face parameterisations requires special treatment. An approach for dealing with the sign conflict problem for unstructured tetrahedral meshes has been presented by Ainsworth and Coyle [1] where two reference tetrahedra are defined and each element is characterised by one of these two.

Unfortunately, the extension of such an approach to hexahedra is not straightforward. The current deal.II [4] finite element library includes a hexahedral H(curl)-conforming finite element which does not fully overcome the sign conflict problem and is only guaranteed to perform correctly on rectangular-based meshes which conform to a standard orientation.

Schöberl and Zaglmayr [2, 3] have proposed an alternative method for overcoming the sign conflict problem which is based upon the definition of global edge and face orientations and the run-time generation of the associated elemental basis functions. We present an implementation of this technique within the deal.II framework and shall present a range of interesting benchmarks, which demonstrate the extension of deal.II's capabilities for the solution of electromagnetic problems on general geometries.

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### A New Scientific Computing Platform on Mobile Devices

**Mark S.K. Lau** *(Hong Kong Baptist University)*

In recent years, advancement of mobile technology opens up new possibilities for scientific computing. Mobile devices become increasingly powerful and have desktop class processor architectures. Numerical libraries such as BLAS, LAPACK, and OpenGL are now optimized for mobile devices. However, popular platforms, such as Matlab and Octave, so far do not have a mobile app that performs computation on local devices. Their existing apps only perform computation on the cloud and results are delivered to the users through the internet. These apps have limited capability and do not make full use of the benefits offered by the mobile platform.

Over the past few years, we have been developing a new computation platform on iPad, known as SIMO, which performs computation entirely locally on mobile devices. It is a truly mobile app that can be used completely offline without losing any of its features and computation power. It uses Matlab syntax, so that scripts created using the app can also be run on Matlab with no or very little modification. It has now more than 120 built-in functions, including frequently used functions for matrix manipulation, linear algebra, random number generators, and probability distributions. SIMO is a fully-fledged platform that features an editor with syntax highlight and auto-indent, a file system for managing user-created scripts, a command prompt, and a plot area for 2D and 3D graphics supporting multi-touch interactions (panning, zooming, and rotation).

This talk can be divided into three parts: First, we introduce major features of SIMO and its basic architecture. Second, we show that SIMO can be a valuable tool for both teaching and learning of numerical subjects. This is accomplished by live demonstrations of some examples taken from textbooks. We share some of our experiences of using SIMO for teaching numerical subjects in a mathematics department. Finally, we discuss the potential of SIMO as a scientific research tool. We conclude by discussing the possibility of developing SIMO into a mobile computing laboratory, which can be used as an integrated environment to analysis and visualize data collected in real time from a mobile device's built-in sensors (such as cameras, gyroscope, GPS, and accelerometer).

### A parallelizable preconditioner for all-at-once solution of time-dependent PDE-constrained optimization problems

**Eleanor McDonald** & Andy Wathen *(Oxford University)*

The study of PDE-constrained optimization problems is becoming an increasingly important area for applied mathematicians and numerical analysts. For parabolic PDEs, an all-at-once approach aims to solve all time-steps in one coupled computation and results in exceedingly large linear systems. In order to solve these systems, we require efficient iterative methods incorporating appropriate preconditioners. Furthermore, the ability of these iterative methods to utilize modern parallel computer architectures provides a significant advantage.

In this talk, we will discuss the solutions to the heat and convection-diffusion control problems. We introduce a new Schur complement based preconditioner

for the resulting saddle-point system. This preconditioner is optimal with respect to the mesh parameter and in addition, it is parallelizable over time which can provide significant speed-up to the computation.

We provide details of the model problems considered and derive the all-at-once linear systems. We will then motivate the preconditioner and illustrate its parallel capabilities. We will also present numerical results to demonstrate the effectiveness of this preconditioner.

**A Computational Model for the Coupled Solution of Reaction-Diffusion Equations on Evolving Domains and Surfaces**

**John Mackenzie**, Grant MacDonald, Michael Nolan *(Strathclyde University)* & Robert Insall *(Beatson Institute for Cancer Research, Glasgow)*

In this talk I will present details about a moving mesh finite element method for the approximate solution of partial differential equations on an evolving bulk domain in two dimensions, coupled to the solution of partial differential equations on the evolving domain boundary. Problems of this type occur frequently in the modeling of eukaryotic cell migration and chemotaxis - for these applications the bulk domain is either the interior or exterior of the cell and the domain boundary is the cell membrane. Fundamental to the success of the method is the robust generation of bulk and surface meshes for the evolving domains. For this purpose we use a moving mesh partial differnetial equation (MMPDE) approach. The developed method is applied to model problems with known solutions which indicate second-order spatial and temporal accuracy. The method is then applied to a model of the two-way interaction of a migrating cell with an external chemotactic field.

**New developments for exact quadrature in $n$-dim Galerkin BEM on polyhedral surfaces**

**Matthias Maischak** *(Brunel University)*

We show a fully analytic quadrature method for the $n$-dimensional Galerkin boundary element method for all standard kernels and arbitrary polynomial degrees on generalized elements using recurrence formulas. Generalized elements are polyhedral subsets with planar faces and are not restricted to triangles. The method is based on the Gauss theorem and the invariance of the standard kernels (or components of standard kernels) with respect to some special first and second order differential operators.

We discuss a model implementation in the form of a software library. Numerical results for some selected examples will be presented which illustrate the feasibility of the exact quadrature method in 3 dimensions.

**An efficient solver for elliptic PDEs on the torus based on trigonometric collocation**

**Dennis Merkert** & Matthias Kabel & Matti Schneider *(University of Kaiserslautern, Germany)*

The solution of elliptic PDEs with periodic boundary conditions is required in many applications, for example in homogenization problems. There, one wants to compute the effective properties of a composite regarding its elastic behavior or heat conductivity.

To solve such problems, Moulinec and Suquet proposed in 1994 an algorithm to solve a Fredholm integral equation of the second kind, equivalent to the equations of linear elasticity, the so-called Lippmann-Schwinger equation. This equation is of the form

$$\epsilon = \epsilon_0 + \Gamma^0 * (C - C^0)\epsilon$$

and describes the strain $\epsilon$ in terms of the piecewise constant stiffness distribution $C$, a constant reference stiffness $C^0$, the macroscopic strain $\epsilon_0$ and the kernel $\Gamma^0$.

The proposed algorithm is based on collocation with trigonometric polynomials and makes heavy use of the fast Fourier transform and its inverse to diagonalize the occurring operators. In this talk, we will present a new derivation and understanding of this algorithm.

Further, we developed an approach to reduce — and in some special cases completely remove — the error introduced by not representing interfaces correctly. This method is based on the theory of laminates and works by smoothing the coefficients near discontinuities. This leads to an error reduction of one order of magnitude in coefficient ranges relevant in applications.

**An introduction to time-dependent Fuzzy Domain Decomposition Methods**

**Jérôme Michaud** *(Edinburgh University)*

In many multiscale physical systems, the use of a single fine-grained model in the complete computational domain is often prohibitively expensive and one has to rely on approximations on at least parts of the domain. This leads to the use of heterogeneous domain decomposition methods.

In the case where it is *a priori* known where which approximation can be used, one can choose appropriate

transmission conditions to obtain an accurate global approximation. However, there are other systems in which the boundaries between the different regions are not *a priori* known and can even change during the simulation. There is a need for new numerical strategies able to change the domain in which one approximation is used adaptively during the simulation. This can be achieved using the so-called Fuzzy Domain Decomposition Methods (FDDMs) introduced in [2] and studied in [1] and in [3].

So far, the FDDMs have been studied with a static decomposition of the domain. In this talk I want to generalize FDDMs to time-dependent problems as it has been done in [3] and demonstrate that these methods are able to dynamically adapt the subdomains in which a particular approximation is used. As an example, I will focus on a 1D example of an advection-dominated problem.

As will be discussed, the local adaptation process is challenging and often problem-dependent. We will also shortly discuss the direction in which this work can be extended.

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**Adaptive hybrid Montecarlo simulated annealing**

**M.J. Moreta** *(Universidad Complutense de Madrid)* & B. Cano *(Universidad de Valladolid)*

In this talk we present an adaptive implementation of hybrid Montecarlo simulated annealing in order to find the global minimum of a given regular function.

In the literature, there exist several algorithms that can be used when searching for the global minimum of a given regular function. In this way, one possibility is to use the classical Newton method to approximate the zero of the gradient of the function. This method is very competitive when the initial iterant converges to the global minimum. However, this method does not guarantee this convergence.

Another alternative is to use a class of simulated annealing algorithms (**SA**), for which there exists several results concerning convergence theorems [1, 3, 4]. These results include the choice of the usually called 'cooling schedule', which is the selection of the values of the temperature in a diminishing way, in order to try to get to the minimum of the given function in the most efficient way. On the one hand, the temperature must diminish slowly so that there is not a big difference among the targeted distributions. On the other hand, the smaller the temperature, the spikier the densities around the global minimum which we are searching.

In this way, following the ideas in [2], we have centered our attention in hybrid Montecarlo simulated annealing (**HSA**), because with this technique, it is possible to use an exponential decaying annealing schedule, which is not of use with other SA methods. Because of this, HSA works better than other standard simulated annealing algorithms in many problems. However, in [2], there is no analysis which justifies the good behaviour of HSA. We present an adaptive code in which we theoretically justify the values of the temperature and the stepsize of hybrid Montecarlo, that are changed at each iteration in order to try to find the minimum of the function with the least number of iterations and rejections. In this manner, despite a precise theorem of convergence with such an adaptive code not given, the numerical results indicate that there exists a rapid convergence at least to a local minimum. Besides, the range of initial iterants which lead to a global minimum is much bigger than with the classical Newton method.

We have implemented two variants of our technique in several examples of functions with several critical points, comparing with the technique in [2] and with the classical Newton method. In this way, it is shown that one of those variants is in general the best, in the sense that more initial iterants converge to the global minimum with the fewest iterations.

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### A Family of Variable Mesh Methods for Solving Higher order Singular Non-linear Boundary Value Problems

**Sucheta Nayak** & Arshad Khan *(Lady Shri Ram College for Women, University of Delhi, INDIA, Jamia Millia Islamia, Delhi, INDIA)*

In this paper, we propose two numerical methods to solve higher order linear and non-linear boundary value problems of the type $u^{(4)} = f(x, u, u^{(1)}, u^{(2)}, u^{(3)})$, $x \in [0, 1]$ with boundary conditions $u(0) = A_1, u^{(2)}(0) = A_2$ and $u(1) = B_1 u^{(2)}(1) = B_2$ where $f \in C^4[0, 1]$ and $A_i$ and $B_i$ are real constants. Second and third order convergence of both the methods have been briefly discussed. Numerical results are also provided to confirm the accuracy and efficiency of the proposed methods.

*Keywords*: Variable mesh, Singular, Non-linear, RMS errors.

### An algorithm to compute the polar decomposition of a $3 \times 3$ matrix

Nicholas J. Higham & **Vanni Noferini** *(University of Manchester)*

When designing algorithms for dense numerical linear algebra problems, we usually look for asymptotic efficiency for *large* values of the dimension, $n$: for instance, we prefer an $\mathcal{O}(n^3)$ flops algorithm to an $\mathcal{O}(n^4)$ one, or we favour algorithms rich in matrix-matrix operations. However, there is a class of problems that is not often considered but is practically important: to solve a large number of very *small* problems.

A small problem needs a different approach: the exponent and constant of the highest order term in the flop count do not necessarily identify the most efficient algorithm, as that term may not dominate; and the prevalence of matrix-matrix operations is also not very meaningful.

We propose an algorithm for computing the polar decomposition [1] of a $3 \times 3$ real matrix that is based on the connection between orthogonal matrices and quaternions [2]. An important application is to 3D transformations in the level 3 Cascading Style Sheets specification used in web browsers. Our algorithm is numerically reliable and requires fewer arithmetic operations than other methods, such as computing the polar decomposition via the singular value decomposition [1], by Newton's method [1], or by the QR-based dynamically weighted Halley iteration [3].

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### Interpretation of the algebraic error in numerical solution of PDEs

**Jan Papež** & Zdeněk Strakoš *(Charles University in Prague)*

In the adaptive numerical solution of PDEs, local mesh refinement is used together with a posteriori error analysis in order to equilibrate the discretization error over the domain. Since the discretized algebraic systems are not solved exactly, one should take into consideration the error caused by the inexact algebraic computation; see, e.g., [3, 1, 5] and the references given there. In particular, the consideration should include the spatial distribution of the algebraic error in the domain; cf. [4].

In the finite element method (FEM) the finite dimensional subspaces are typically generated using locally supported basis functions. Elaborating on [2, 4], we present the idea of interpreting the algebraic error as a transformation of the discretization basis. We will see that the resulting transformed basis is of global support. Second, we present the generalization of the discrete Green's function for a computed approximation and use it for expressing the algebraic error.

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### Splitting methods for the time integration of the Klein-Gordon equation with Hagstrom-Warburton high-order absorbing boundary conditions

**A.M. Portillo** & I. Alonso-Mallo *(Universidad de Valladolid)*

The Klein-Gordon equation on an unbounded one dimensional domain is considered. Numerical computation is reduced to a finite domain by using the Hagstrom-Warburton (HW) high-order absorbing boundary conditions (ABCs). A fourth order finite difference discretization in space is used. Time integration is made by a fourth order splitting method which is efficient and easy to implement. The splitting method proposed permits refinement of the full discretization to study the behavior of the absorption error. The performance of H-W ABCs when the dispersion coefficient varies is considered. Numerical experiments displaying the improvement in the accuracy of the numerical solution are provided.

### An optimal solver for linear systems arising from stochastic FEM approximation of diffusion equations with random coefficients

**P Pranjal** & David Silvester *(University of Manchester)*

This talk discusses the design and implementation of efficient solution algorithms for symmetric linear systems associated with stochastic Galerkin approximation of elliptic PDE problems with correlated random data. The novel feature of our preconditioned MINRES solver is the incorporation of error control in the natural "energy" norm in combination with an effective a posteriori estimator for the PDE approximation error. This leads to a robust and optimally efficient stopping criterion: the iteration is terminated as soon as the algebraic error is insignificant compared to the approximation error.

### Finite element methods for coupling bulk and surface phenomena

**Thomas Ranner** *(University of Leeds)*

Natural phenomena domained by both bulk and surface affects arise in many natural situations including alloy solidification and cell biology. In this talk I will give details of two finite element methods for numerically approximating the solution of a bulk partial differential equation coupled to a surface partial differential equation. The first is a *fitted finite element method*, previously presented by [C.M. Elliott and T. Ranner, *IMA J. Numer. Anal. 33(2) (2013), pp. 377–402.*]. The key idea is to take a polyhedral approximation of the bulk region, consisting of a union of simplices, and to use the piecewise polygonal boundary faces as an approximation of the surface. Two finite element spaces are defined, one in the bulk region and one on the surface, consisting of piecewise linear functions with respect to the given subdivisions. The second method is a new *unfitted finite element method*. The bulk domain is embedded in a polyhedral domain consisting of simplices. The underlying feature of the method is that the finite element approximation space is based on piecewise linear finite element functions on the embedded triangulation which is independent of the bulk domain or the surface. On the surface, the full gradient is used rather than the projected tangential gradient which distinguishes our unfitted method for the method of [S. Gross, M.A. Olshanskii and A. Reusken, *arXiv preprint* arXiv:1406.7694]. Both methods are presented for a model elliptic problem. A priori analysis is presented first using an abstract framework which is applied to both methods. A numerical implementation is used to demonstrate that analytical properties are observed in practice and the applicability of both methods to a variety of situations. Finally, I will discuss how these approaches (and the numerical analysis) may be generalised to the evolving case.

### Meshfree methods for Brinkman flows driven by arbitrary forces

**Magda Rebelo** & Nuno F.Martins *(UNL, Portugal)*

In this work we consider an interior boundary value problem for the Brinkman system

$$\begin{cases} (\Delta - \lambda)\mathbf{u} - \nabla p = \mathbf{f} & \text{in } \Omega, \\ \nabla \cdot \mathbf{u} = 0 & \text{in } \Omega, \\ \mathcal{B}(\mathbf{u}, p) = \mathbf{g} & \text{on } \Gamma = \partial\Omega \end{cases} \tag{3}$$

where $\lambda > 0$ is constant.

We shall consider two boundary conditions:

Dirichlet type boundary condition

$$\mathcal{B}(\mathbf{u}, p) = \mathbf{u}|_\Gamma; \tag{4}$$

Neumann type boundary condition

$$\mathcal{B}(\mathbf{u}, p) = T(\mathbf{u}, p)\mathbf{n}|_\Gamma, \tag{5}$$

where the traction boundary operator $T$ is defined in terms of the stress tensor associated to the flux $(\mathbf{u}, p)$, $T(\mathbf{u}, p) = -pI + \nabla\mathbf{u} + \nabla\mathbf{u}^\top$.

In order to obtain a numerical solution of these problems we propose a meshfree method. We start by studying the homogeneous problems. Here, we give theoretical results concerning approximations using fundamental solution basis functions. For the non-homogeneous case, we consider the method of particular solutions. In this well known method, the problem is decomposed in two problems: one for finding a particular solution, and the other for solving a homogeneous problem. We propose a representation for the fluid flow as a linear superposition of unsteady Stokeslets and elastodynamic P and S waves. A theoretical study for the proposed choice of basis functions is given and several numerical examples are presented in order to illustrate and discuss the feasibility of the method.

**Sparse Galerkin BEM for the heat equation**

**Anne Reinarz** *(University of Reading)* & Alexey Chernov *(University of Oldenburg)*

The numerical solution of parabolic time evolution problems such as the heat equation is required in numerous applications. Solving this problem using the boundary element method (BEM) is an attractive alternative to traditional methods, such as Finite Elements combined with a time-stepping scheme.

In this talk we discuss combining BEM with anisotropic sparse tensor product bases that can yield improved convergence rates. This is expected to reduce the total work to $O(h^{-(d-1)})$, where $d$ is the spatial dimension and $h$ is the spatial mesh width.

Using BEM generally leads to full systems, so we combine it with a wavelet method. This leads to sparse system matrices that can be solved in linear complexity. The theoretical results are supported by numerical experiments.

**Taylor's Theorem for Matrix Functions and Pseudospectral Bounds on the Condition Number**

**Samuel D. Relton** & Edvin Deadman *(The University of Manchester)*

This talk describes how we can generalize Taylor's theorem from complex scalar functions $f\colon \mathbb{C} \to \mathbb{C}$ to matrix functions $f\colon \mathbb{C}^{n\times n} \to \mathbb{C}^{n\times n}$ such as the matrix exponential and logarithm, obtaining the remainder term explicitly as a contour integral. More precisely we prove that

$$\begin{aligned} f(A+E) &= \sum_{j=0}^{k} \frac{1}{j!} D_f^{[j]}(A,E) + \frac{1}{2\pi i}\int_\Gamma f(z) \\ &\qquad (zI - A - E)^{-1}[E(zI-A)^{-1}]^{k+1} dz \\ &\equiv T_k(A,E) + R_k(A,E), \end{aligned}$$

where $T_k(A,E)$, the Taylor polynomial, is the summation of the $D_f^{[j]}(A,E)$ terms (representing the $j$th Fréchet derivative of $f$ in the direction $E$) and $R_k(A,E)$ is the remainder expressed via a contour integral.

We use this result to investigate the behaviour of the condition number of a matrix function: its sensitivity to small perturbations in the input. The condition number is defined as

$$\mathrm{cond}(f,A) = \lim_{\epsilon\to 0} \sup_{\|E\|\le\epsilon\|A\|} \frac{\|f(A+E) - f(A)\|}{\epsilon}.$$

Applying techniques borrowed from the study of pseudospectra to the remainder term we can obtain upper bounds on the condition number of the matrix function. In particular we show that

$$\mathrm{cond}(f,A) \le \frac{L_\epsilon}{2\pi\epsilon^2} \max_{z\in\Gamma_\epsilon} |f(z)| \frac{\|A\|}{\|f(A)\|},$$

where $L_\epsilon$ is the length of a contour $\Gamma_\epsilon$ enclosing the $\epsilon$-pseudospectrum of $A$.

Focusing on the matrix function $f(A) = A^t$ for $t \in (0,1)$ and using a keyhole contour allows us to bound the condition number in the Frobenius norm by

$$\mathrm{cond}(x^t,A) \le \frac{2(\pi+1)\rho_\epsilon^{1+t}}{2\pi\epsilon^2} \frac{\|A\|_F}{\|f(A)\|_F},$$

where $\rho_\epsilon$ is the pseudospectral radius for some given $\epsilon$. Our numerical experiments show that this upper bound on the condition number can be calculated extremely efficiently, obtaining a 900x speedup over the current state-of-the-art method in some cases. The price paid for this speed is that the bound can be rather weak, meaning that one might wish to revert to the current method when a more accurate estimate of the condition number is required.

**Parallelised Adaptive Importance Sampling**

**Paul Russell** & Colin Cotter, Simon Cotter *(University of Manchester)*

It is frequently of interest to solve data assimilation problems of the form

$$D = \mathcal{G}(u) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0,\Sigma),$$

where the data $D$ is a noisy observation of the system $\mathcal{G}(u)$. We assume knowledge of the observation operator $\mathcal{G}$, and the covariance operator for the noise, $\Sigma$, and try to recover the parameter $u$ which best satisfies the equation.

Viewing the problem from a Bayesian perspective and assuming prior knowledge of $u \sim \mathcal{N}(0, \mathcal{T})$ we can construct a posterior distribution, $\mu_Y$, and use Markov Chain Monte Carlo (MCMC) to produce a sample from this distribution. I will demonstrate that commonly used serial MCMC methods do not take full advantage of modern computer architecture, and that designing parallel algorithms can lead to a large reduction in computational costs.

### A posteriori error analysis of discontinuous Galerkin methods for elliptic interface problems

**Younis Sabawi** (jointly with Manolis Georgoulis) & Andrea Cangiani *(University of Leicester)*

We present a residual-based a posteriori error estimator for interior penalty discontinuous Galerkin methods applied to the solution of elliptic interface problems modelling the mass transfer of solutes through a semi-permeable membrane. The posterior error bound is derived under the assumption that the triangulation is aligned with the interfaces and choosing appropriate numerical fluxes at the inter-element boundaries that are on the interface. Upper and lower bounds of the error are proved in terms of the energy norm. Numerical experiments highlighting the performance of the proposed method are presented.

### Analysis of the convergence of Convolution Quadrature type methods

**Nicolas Salles** & Timo Betcke *(University College London)*

Convolution Quadrature (CQ) methods are Laplace transform type methods for the solution of time-domain wave problems using Boundary Integration Equations. This method is quite recent since it was introduced by C. Lubich in 1988 [1,2] but the method was already widely studied [3, 4, 5] for example. A benefit of this method is that it is fully parallelizable since it requires to solve independent frequency problems and so an existing frequency solver code can easily be used for the implementation.

This talk provides several new analytical results on the convergence of the numerical solution of acoustic problems computed using a CQ method. CQ methods relies upon an implicit A-stable time discretization scheme, usually multistep scheme (backward Euler, BDF-2 ...) or stiffly accurate Runge-Kutta scheme (RadauIIa, LobattoIIIc ...). The number of frequency problems solved is generally identical to the number of time steps.

We study what happens when we decouple the number of frequency solves from the number of time steps and specifically the convergence of the numerical solution obtained with a CQ method to the exact solution of the wave equation obtained with the underlying time discretisation scheme when the number of frequency problems solved increases. Error estimates are obtained using results on the convergence of trapezoidal rule [7] and the location of the scattering poles [6] for multistep rules. The influence of the integral formulation on the rate of convergence to the exact solution of the underlying time discretization scheme is also studied. Finally, the extension of the convergence results to Runge-Kutta Convolution Quadrature methods is briefly introduced. Numerical examples computed with BEM++ [8] using multistep and Runge-Kutta schemes for the scattering by the unit sphere and by some trapping domains will be presented.

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### Symmetric Interior Penalty Galerkin (SIPG) Method with Average Vector Field Method (AVF) for Cahn–Hilliard System with Degenerate Mobility

**Ayşe Sarıaydın** & Murat Uzunca & Bülent Karasözen *(Middle East Technical University, Turkey)*

The Cahn–Hilliard (CH) equation is a central model introduced by Cahn and Hilliard to describe the phase separation and coarsening phenomena in a melted alloy [3]. Recently, it has been used to model many moving interface problems from fluid dynamics to material science using phase–field approach.

In this contribution, we consider the Cahn–Hilliard system with the degenerate mobility function in [6]. In order to capture the physical properties of this system discontinuous Galerkin finite elements method (DGFEM) [1, 5] is coupled with average vector field (AVF) method. The DGFEM approximation allows us to capture the sharp gradients or singularities that affect the numerical solution locally. AVF method [2, 4] is the only second order implicit energy stable and structure preserving integrator. It preserves the energy for gradient systems and for systems with Lyapunov functions. The unconditional energy stability of the fully discrete scheme is also proven and supported with some numerical results.

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### Solving FEM/BEM Coupled Problems With FEniCS And BEM++

**Matthew Scroggs**, Timo Betcke & Erik Burman *(University College London)*

Boundary element simulations are frequently used within engineering to simulate problems in homogeneous unbounded domains, for example acoustic scattering from a car. However, in many realistic applications small localised inhomogeneities can appear. In these situations, it is necessary to couple FEM and BEM subproblems efficiently.

In recent years we have developed at UCL a fast boundary element package called BEM++ which provides a simple Python interface based on a fast C++ computational kernel. In this talk we discuss efforts and first examples of interfacing BEM++ with FEniCS, a popular FEM library, for coupled FEM/BEM simulations. The goal is to provide a simple but powerful Python based framework to setup and solve challenging FEM/BEM coupled problems in a variety of applications.

### A high order method for advection dominated problems with fractional diffusion

**Ercília Sousa** *(University of Coimbra)*

Fractional derivatives have been used to model anomalous diffusion and recently the fractional advection diffusion equation has been presented as a suitable model for many problems that appear in different fields, such as biology, finance and hydrology. This equation can be obtained from the standard advection diffusion equation by replacing the second order spatial derivative by a fractional operator of an order between one and two. This operator is defined by a combination of the left and right Riemann-Liouville derivatives.

We propose a high order explicit numerical method for solving fractional advection diffusion problems. For the particular case, when the fractional operator is of order two, leading to the second order derivative, this method matches the numerical method QUICKEST. The convergence of the numerical method is studied through consistency and stability. The order of convergence varies between two and three and for advection dominated flows is close to three. Although the method is conditionally stable, the restrictions allow wide stability regions. Some numerical experiments will be presented to show the performance of the method and to observe the anomalous diffusion.

### Applying GMRES to the Helmholtz equation with shifted Laplacian preconditioning: what is the largest shift for which wavenumber-independent convergence is guaranteed?

**Euan Spence** & Martin Gander & Ivan Graham *(University of Bath)*

There has been much recent research on preconditioning discretisations of the Helmholtz operator $\Delta + k^2$

using a discrete version of the so-called "shifted Laplacian" $\Delta + (k^2 + i\varepsilon_M)$ for some $\varepsilon_M > 0$. This is motivated by the fact that, as $\varepsilon_M$ increases, the shifted problem becomes easier to solve iteratively. Despite many numerical investigations, there has been little rigorous analysis of how to choose the shift.

In this talk, we focus on the question of how large $\varepsilon_M$ can be so that the shifted problem provides a preconditioner that leads to $k$-independent convergence of GMRES, and our main result is a sufficient condition on $\varepsilon_M$ for this property to hold. Note that we do not address the important question of how large $\varepsilon_M$ should be so that the preconditioner can easily be inverted by standard iterative methods – this is discussed for domain decomposition preconditioners in the talk by Ivan Graham.

### Selective Segmentation with Intensity Inhomogeneity

**Jack Spencer** & Ke Chen *(University of Liverpool)*

In the field of imaging sciences, segmentation in the variational framework is the task of partitioning a given image function into subregions. Automatic segmentation is a challenging task and achieving robustness is a major problem, especially in the context of selective segmentation. The two-phase piecewise-constant case of the Mumford-Shah formulation (2PCMS) is most suitable for images with simple and homogeneous features where the intensity variation is limited. However, it has been applied to many different types of synthetic and real images after some adjustments to the formulation. Recent work has incorporated user input into variational models to isolate objects within an image with some success, however many require nonconvex minimisation and therefore provide inconsistent results.

This talk addresses the task of generalising the 2PCMS model to account for intensity inhomogeneity which is common for real life images. We first review existing methods for treating inhomogeneity and demonstrate inconsistencies in these methods. We propose a modified variational model to account for these problems by introducing additional constraints, and extend this concept to selective segmentation with the introduction of a distance selection term. These models are minimised with convex relaxation methods, where the global minimiser can be found for a fixed fitting term. We also present an improved additive operator splitting method, that is consistent with the convex relaxation framework. Finally, we present numerical results that demonstrate an improvement to existing methods in terms of reliability, and results for our new method for selective segmentation.

### ADI method for two-dimensional pseudo-parabolic equation with integral boundary conditions

**Artūras Štikonas** & Mifodijus Sapagovas & Olga Štikonienė *(Vilnius University)*

We consider the third order linear pseudo-parabolic equation in a rectangle with nonlocal integral boundary conditions in one direction and Dirichlet boundary conditions in another direction. Pseudo-parabolic equations with nonlocal boundary conditions arise from various physical phenomena, particularly, the dynamics of ground moisture. A very close mathematical model arises in the study of the incompressible non-Newtonian flow problem.

We provide a numerical algorithm based on the Peacemen-Rachford alternating direction implicit (ADI) method [1]. According to this algorithm it is necessary to solve alternately two systems of difference equations with tridiagonal matrices, one of these systems is solved with nonlocal conditions [2]. Each of the systems is a three-layer difference scheme and it approximates the initial problem with truncation error $\mathcal{O}(\tau + h^2)$.

For investigation of stability of this method we rewrite the three-layer scheme in an equivalent form of a two-layer scheme $\mathbf{Y}^{n+1} = \mathbf{S}\mathbf{Y}^n$, where $\mathbf{Y}^n$ is a vector defined on two layers, $\mathbf{S}$ is a nonsymmetric matrix. The stability conditions are derived by investigating the spectrum of $\mathbf{S}$. To this end, we analyse the auxiliary nonlinear eigenvalue problem.

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### A way to improve incremental 2-norm condition estimation

**Jurjen Duintjer Tebbens** & Miroslav Tůma *(Academy of Sciences of the Czech Republic)*

In 1990, Bischof introduced an estimator for the 2-norm condition number of triangular matrices which is incremental [1], i.e. which computes the estimate of a leading principal submatrix of size $k$ from a cheap update of the estimate for the leading principal submatrix of size $k-1$. It is therefore very suited for usage in (incomplete) factorizations, where columns or rows are computed one-by-one. A very similar estimator,

using approximate right singular vectors instead of approximate left singular vectors, was proposed by Duff and Vömel in 2002 [2]. It has some advantages over Bischof's estimator for sparse matrices, but appears to perform alike with dense matrices.

In this talk we present some new comparisons of the two techniques, which reveal that the main strength of Duff and Vömel's estimator is in approximating the maximum singular value. This can be exploited when the inverse of the triangular matrix is computed simultaneously, which is the case in some decompositions. This leads to a cheap and highly accurate estimator [6], potentially useful in incomplete factorization techniques, where robust dropping and pivoting rules rely on monitoring the condition numbers of the submatrices that are consecutively constructed [2, 3, 4].

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## The design of a fast boundary element method for use in medical ultrasound techniques

**Elwin van't Wout**, Timo Betcke, Pierre Gélat & Simon Arridge *(University College London)*

The conventional medical treatments of liver cancer are invasive procedures such as surgical resection, which pose severe health risks to the patients. As a non-invasive alternative, high-intensity focused ultrasound (HIFU) can be used to ablate tumours by heating a localised region of tissue. In the case of HIFU treatment of liver cancer, the scattering of ultrasound by ribs can result in overheating of the bone and abberations at the focal region. The patient-specific planning for transcostal HIFU treatment is likely to rely on numerical modelling to optimise the multi-element array of ultrasound transducers [1].

Typical HIFU configurations operate at MHz frequencies and therefore result in large-scale scattering problems. This paper aims to design a fast boundary element method (BEM) specifically for transcostal HIFU treatment planning. Firstly, the Galerkin discretised Burton-Miller formulation is used, which is devoid of resonances. Secondly, compression techniques based on data-sparse $\mathcal{H}$-matrix representations significantly reduce the memory footprint. Thirdly, quick convergence of the iterative linear solver is achieved with operator preconditioning based on a high-frequency approximation of the Neumann-to-Dirichlet map with on-surface radiation conditions [2]. Because the preconditioner is sparse and accurate for high-frequency scattering, it significantly reduces the number of iterations while adding only little overhead.

The fast BEM has been implemented in the open-source library `BEM++` [3]. Its feasibility for the use in medical ultrasound techniques has been demonstrated experimentally. Efficient simulations have been achieved for the acoustic scattering analysis of a multi-element transducer array that focuses the ultrasound field of 1 MHz behind a human ribcage model.

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## Stabilization of High Aspect Ratio Mixed Finite Elements for Incompressible Flow

**Andreas Wachtel** & Mark Ainsworth & Gabriel R. Barrenechea *(University of Strathclyde)*

Anisotropic refinement is an interesting concept to resolve local features of solutions. Unfortunately, the stability of a mixed finite element method may depend on the aspect ratio and other mesh properties caused by the refinement. For an arbitrary order pair with discontinuous pressures, we show which part of the pressure space is responsible for the deterioration of stability. By imposing a minimal amount of constraints on the pressure, two mixed methods circum-

venting the behaviour arise. Numerical experiments confirm their stability.

### Efficient Numerical Methods for Solar Corona Simulations

**Marion Weinzierl** & Anthony Yeates *(Durham University)*

Making solar magnetohydrodynamic simulations as fast as possible is crucial for relevant and accurate prediction of space weather events that will affect the Earth. To efficiently model the build up of electric currents in the corona, we combine the magneto-frictional method, which is known to provide good predictions of the behaviour of the solar corona in real-time, with efficient multigrid methods for determining the photospheric electric field from line-of-sight photospheric magnetograms. As this only gives us the inductive part of the electric field, which differs significantly from the complete field, additional physical assumptions or observations (which are in general not openly available) are usually used to estimate the missing component. One can, however, observe that the deviation from the expected electric field depends significantly on the differential rotation, i.e., if we "switch off" the differential rotation in our simulations, the approximation of the electric field without the inductive component has a much smaller error than the simulation including this large-scale flow. Consequently, we propose to deduce the non-inductive electric field from the known differential rotation.

By using a special form of uniformly spaced curvilinear coordinates we are able to solve the respective equations on a Cartesian grid by only adapting the righthand sides. This improves the efficiency and robustness of the multigrid solver compared to a solver on a curvilinear grid.

### Fractional Allen-Cahn Equations

**Hamdullah Yücel** & Martin Stoll & Peter Benner *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*

Fractional differential equations are becoming increasingly used as a modelling tool to describe a wide range of non-classical phenomena in applied science and engineering, for example, anomalous diffusion problems, or the subdiffusion and superdiffusion processes. However, the non-local nature of the factional operators cause the essential difficulties and challenges for numerical approximations. In this talk, we propose an efficient approach to solve fractional-in-space Allen-Cahn equations via the contour integral method (CIM) for computing the fractional power of a matrix times a vector. Time discretization is performed by the first- and second-order implicit-explicit schemes, whereas spatial discretization is performed by discontinuous Galerkin methods. Several numerical examples in two and three dimensions are illustrated to show efficiency of the proposed approach.