24th Biennial Conference on Numerical Analysis

28 June - 1 July, 2011

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Introduction

Dear Participant,

On behalf of the Strathclyde Numerical Analysis Group, it is my pleasure to welcome you to the 24th Biennial Numerical Analysis conference. This is the second time the meeting has been held at Strathclyde and continues the long series of "Dundee Numerical Analysis Conferences".

The conference is rather unique 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, what I hope you will agree is, an impressive line up of eminent plenary speakers.

The conference is funded almost entirely from the registration fees of the participants, augmented with contributions from the *A.R. Mitchell Fund* and the *Gene Golub Fund*. This year, we are grateful to the EPSRC and Scottish Funding Council funded centre for Numerical Algorithms and Intelligent Software (NAIS), for providing funding for some of the invited speakers. 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 find the conference both stimulating and enjoyable, and look forward to welcoming you back to Glasgow again in 2013!

Mark Ainsworth
Conference Chairman

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 conference office will be located in the Cluster Manager's office, room K4.12a of the John Anderson building. 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 K3.26.

- **Meals**. All meals (except lunch on Friday) will be served in the Lord Todd Dining Room (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 K3.25.

- **Lecture rooms**. These are mainly in the John Anderson building (building 16, enter on Level 4 from Taylor Street). The main auditorium (K3.25) is down one floor from the main entrance, along with breakout rooms K3.14, K3.17, K3.26 and K3.27. The additional breakout rooms are K4.12 (on the entrance level of the John Anderson building near the registration desk) and AR201 (in the Architecture building, no. 17 on the campus map). These will be signposted.

- **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!

- **Coffee and tea breaks**. Coffee and tea will be provided at the advertised times in the foyer outside K3.25.

- **Bar**. There is a bar in the Lord Todd building (building 26) next to the dining room.

- **Reception**. A reception for all participants hosted by Glasgow City Council will be held in the City Chambers on Tuesday 28th June from 20.00 to 22.00. The City Chambers is marked on the campus map: entry is from George Square.

- **Conference dinner**. The conference dinner will be held in the Lord Todd Dining Room on Thursday 30th June at 19.00 for 19:30. The guest speaker will be Professor David Silvester, University of Manchester.

- **Book displays**. There will be books on display for the duration of the conference in room K3.26.

- **Internet Access**. Delegates will be provided with a username and password for internet access at registration. Wireless access is available in all of the meeting rooms and in the Lord Todd bar/restaurant. Computer terminals will be available from 09:00-17:00 Tuesday-Thursday in room C3.09 of the Colville Building. This room can be accessed from the John Anderson building past lecture rooms K3.14 and K3.17 and will be signposted.

- **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.

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Abstracts of Invited Talks

Spectral frequency- and time-domain PDE solvers for general domains

Oscar Bruno *(Caltech)*

We present fast frequency- and time-domain spectrally accurate solvers for Partial Differential Equations that address some of the main difficulties associated with simulation of realistic engineering systems. Based on a novel Fourier-Continuation (FC) method for the resolution of the Gibbs phenomenon, associated surface-representation methods and fast high-order methods for evaluation of integral operators, these methodologies give rise to fast and highly accurate frequency- and time-domain solvers for PDEs on general three-dimensional spatial domains. Our fast integral algorithms can solve, with high-order accuracy, problems of electromagnetic and acoustic scattering for complex three-dimensional geometries; our FC-based differential solvers for time-dependent PDEs, in turn, give rise to essentially spectral time evolution, free of pollution or dispersion errors. A variety of applications to linear and nonlinear PDE problems demonstrate the very significant improvements the new algorithms provide over the accuracy and speed resulting from other approaches.

On the Future of High Performance Computing: How to Think for Peta and Exascale Computing

Jack Dongarra *(University of Tennessee)*

In this talk we examine how high performance computing has changed over the last 10-year and look toward the future in terms of trends. These changes have had and will continue to have a major impact on our software. Some of the software and algorithm challenges have already been encountered, such as management of communication and memory hierarchies through a combination of compile–time and run–time techniques, but the increased scale of computation, depth of memory hierarchies, range of latencies, and increased run–time environment variability will make these problems much harder.

We will look at five areas of research that will have an importance impact in the development of software and algorithms.

We will focus on following themes:

- Redesign of software to fit multicore and hybrid architectures
- Automatically tuned application software
- Exploiting mixed precision for performance
- The importance of fault tolerance
- Communication avoiding algorithms

Image-Based Biomedical Modeling, Simulation and Visualization

Chris Johnson *(University of Utah)*

Increasingly, biomedical researchers need to build functional computer models from images (MRI, CT, EM, etc.). The"pipeline" for building such computer models includes image analysis (segmentation, registration, filtering), geometric modeling (surface and volume mesh generation), large-scale simulation (parallel computing, GPUs), large-scale visualization and evaluation (uncertainty, error). In my presentation, I will present research challenges and software tools for image-based biomedical modeling, simulation and visualization and discuss their application for solving important research and clinical problems in neuroscience, cardiology, and genetics.

Numerical Methods for Large Scale Inverse Problems in Image Reconstruction

James Nagy *(Emory University)*

One of the most difficult challenges in numerical analysis is the development of algorithms and software for large scale ill-posed inverse problems. Such problems are extremely sensitive to perturbations (*e.g.* noise) in the data. To compute a physically reliable approximation from given noisy data, it is necessary to incorporate appropriate regularization (i.e., stabilization) into the mathematical model. Numerical methods to solve the regularized problem require effective numerical optimization strategies and efficient large scale matrix computations.

In this talk we describe how the challenges of solving linear inverse problems can be analyzed using the singular value decomposition, and how to efficiently implement the ideas with iterative methods on realistic large scale problems. We also discuss how the approaches can be adapted for use on nonlinear inverse problems. Applications from medical imaging will be used for illustration.

Optimization Methods for Machine Learning

Jorge Nocedal *(Northwestern University)*

How good is today's speech recognition software? How are essential features extracted from acoustic frames? What kind of numerical optimization techniques are capable of training a statistical model, using a very large data set, to make accurate predictions on such a difficult problem? I will begin this talk with a real time demonstration of Google's Voice Search to illustrate the progress that has been made in speech recognition, as well as its limitations. This will lead us to the discussion of online vs batch optimization methods, and to some interesting open questions from the perspective of numerical optimization. The main part of the talk will address a claim that is commonly heard in the machine learning community, namely that "the best optimization algorithms are not the best learning algorithms". I will challenge this claim from both a practical and theoretical perspective. I will conclude

the talk by presenting results of two new algorithms on a speech recognition problem provided by Google.

On Computational Strategies for Fluid-Structure Interaction: Some Insights into Algorithmic Basis with Applications

D. Perić & W. Dettmer *(Swansea University)*

This talk is concerned with algorithmic developments underpinning computational modelling of the interaction of incompressible fluid flow with rigid bodies and flexible structures.

Fluid-structure interaction (FSI) represents a complex multiphysics problem, characterised by a strong coupling between the fluid and solid domains along moving and often highly deformable interfaces. Spatial and temporal discretisations of the FSI problem result in a coupled set of nonlinear algebraic equations [1], which is solved by a variety of different computational strategies, ranging from weakly coupled partitioned schemes to strongly coupled monolithic solvers.

This work discusses different options available to the developers focusing on the so-called strongly coupled procedures. Simple model problems are employed to illustrate the algorithmic properties of different methodologies, including a detailed convergence and accuracy analysis. In particular, we investigate the effects of different time integration schemes in the sub-domains of a coupled problem [4]. Furthermore, careful analysis is performed of the coupling strategies and their effect on the convergence of the overall procedure [3].

A comparative analysis between the exact Newton-Raphson methodology and its inexact version is performed on large scale simulations. In particular, we investigate: (i) the effect of the terms that couple the fluid flow with the fluid mesh motion, and (ii) consequences of employing different partitioned strategies on the efficiency and convergence of the overall solution procedure [2].

Numerical examples will be presented throughout the talk in order to illustrate the scope and benefits of the developed strategies.

The examples include analysis of interaction of both external and internal flows with rigid bodies and flexible structures relevant for different areas of engineering including civil, mechanical and bio-engineering.

Mathematical models for the cardiovascular system: analysis, numerical simulation, applications

A. Quarteroni *(Ecole Polytechnique Fédérale de Lausanne and Politecnico di Milano)*

The role of mathematics in understanding and simulating fluid dynamics and biochemical processes in the physiological and pathological functioning of the human cardiovascular system is becoming more and more crucial. These phenomena are indeed correlated with the origin of some major cardiovascular pathologies, and influence the efficacy of the treatments to heal the arteries from their diseases.

Mathematical models allow the description of the complex fluid-structure interaction which govern the

artery wall deformation under the pressure pulse. Moreover, appropriate reduction strategies can be devised to allow for an effective description of the interaction between large, 3D components, and small 1D branches of the circulatory system, as well as the transfer of drugs and chemicals between the arterial lumen and the vessel wall.

This presentation will address some of these issues and a few representative applications.

Kernel-Based Meshless Methods for Solving PDEs

Robert Schaback *(Universität Göttingen)*

I shall focus on numerical methods using trial spaces spanned by functions $K(\cdot, x_j)$ with a symmetric positive definite **kernel** $K : \Omega \times \Omega \to \mathbb{R}$ on a domain $\Omega \subset \mathbb{R}^d$, using finitely many **scattered trial nodes** $x_j \in \Omega$. This setting is independent of PDE solving and can be used for generalized Hermite–Birkhoff interpolation or for approximation, e.g. in Machine Learning.

When these trial spaces are used for PDE solving, they lead to a variety of numerical methods whose common feature is being **meshless**, i.e. not using triangulations and expressing everything "*entirely in terms of nodes*" (Belytschko et. al. 1996).

A first subtopic will be **Trefftz–type methods**, where the kernel–based trial space is **adapted** to the PDE to be solved. For homogeneous problems, this comprises the method of **fundamental** solutions and certain new techniques based on **harmonic kernels**. For inhomogeneous problems, kernel–based trial spaces provide plenty of **particular** solutions. Looking at the error of these methods will lead to a non–roundoff version of a **backward error analysis**.

A second subtopic will focus on PDE–**independent** trial spaces spanned by kernel translates, and provide a framework for error analysis of PDE solving using these trial spaces together with different independent forms of strong or weak testing. This applies to various numerical techniques, including symmetric and unsymmetric meshless collocation and the Meshless Local Petrov–Galerkin method.

Numerical examples will be omitted, since there are plenty of them in the engineering literature. The focus will be on mathematical analysis instead.

The best of fast N-body methods

Robert Skeel *(Purdue University)*

The problem of calculating a sum of pairwise interactions for a large set of particles is not only of great importance for particle simulations but also of great value for continuum simulations. The multilevel summation method (MSM), which does this calculation in linear time, embodies many if not most of the best features of both hierarchical clustering methods (tree methods, fast multipole methods, hierarchical matrix methods) and FFT-based 2-level methods (particle–particle particle–mesh methods,

particle–mesh Ewald methods). Like a hierarchical clustering method (HCM), the MSM parallelizes well and is spatially adaptable. Like FFT-based methods, the MSM is a simple and computes quantities that are continuous as a function of particle positions. The simplicity of MSM is demonstrated by a derivation that approximates the interaction kernel as a linear combination of basis functions and represents this as a sparse matrix decomposition. This is followed by a detailed comparison with HCMs and FFT-based methods and concluded with a summary of recent work concerning performance on graphical processing units and improved approximation schemes.

Error estimates and adaptive algorithms for single and multievel Monte Carlo Simulation of Stochastic Differential Equations

Raul Tempone *(KAUST)*

This talk presents a generalization of the multilevel Forward Euler Monte Carlo method introduced in [1] for the approximation of expected values depending on the solution to an Ito stochastic differential equation [2,3]. The work [1] proposed and analyzed a Forward Euler Multilevel Monte Carlo method based on a hierarchy of uniform time discretizations and control variates to reduce the computational effort required by a standard, single level, Forward Euler Monte Carlo method. Here we introduce and analyze an adaptive hierarchy of non-uniform time discretizations, generated by single level adaptive algorithms previously introduced in [4, 5]. These adaptive algorithms apply either deterministic time steps or stochastic time steps and are based on adjoint weighted a posteriori error expansions first developed in [6]. Under sufficient regularity conditions, both our analysis and numerical results, which include one case with singular drift and one with stopped diffusion, exhibit savings in the computational cost to achieve an accuracy of $O(TOL)$, from $O(TOL^{-3})$ using the single level adaptive algorithm to $O((TOL^{-1}\ \log\ (TOL))^2)$; for these test problems single level uniform Euler time stepping has a complexity $O(TOL^{-4})$.

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Six myths of polynomial interpolation and quadrature

Lloyd N. Trefethen *(University of Oxford)*

Computation with polynomials is a powerful tool for all kinds of numerical problems, but the subject has been held back by longstanding confusion on a number of key points. In this talk I will attempt to sort things out as systematically as possible by identifying six widespread misconceptions. In each case I will explain how the myth took hold — for all of them contain some truth — and then I'll give theorems and numerical demonstrations to explain why it is mostly false.

Finite element approximations for coupled problems

Barbara Wohlmuth *(TU München)*

Numerical simulation of coupled problems play an important role in many different fields. In a wide range of industrial, environmental and medical applications, free-flow and porous media transport processes and elasto-acoustic occur. Although of high relevance, the mathematical modeling and the numerical simulation of complex coupled problems remains challenging. This talk adresses two issues: firstly different areas are illustrated and numerical examples are given. Characteristically for many applications is that the coupling can be realized in terms of balance equations which result in saddle-point like structures. A pair of variables has to guarantee the proper information transfer across the interfaces. In addition to this aspect many complex mathematical models for, e.g., phase transition processes or plasticity involve additional constraints which result in a weak variational inequality setting. In the second part of the talk we review on stable discretization schemes and on optimal a priori estimates for finite element approximations. Here special focus is on the importance of uniform inf-sup stability and the role of surface or volume based Lagrange multipliers.

Minisymposia abstracts

Minisymposium M1
Recent developments in a-posteriori error estimation
Organisers: Gabriel Barrenechea and Richard Rankin

A posteriori error estimation and an adaptive scheme for the choice of the stabilization parameter in low-order finite element approximations of the Stokes problem.

Alejandro Allendes, Mark Ainsworth, Gabriel R. Barrenechea & Richard Rankin *(University of Strathclyde).*

The numerical solution of the Stokes problem can be faced using two complementary approaches. One consists of using classical inf-sup stable pairs of elements. The other consists of stabilizing an inf-sup unstable pair, by adding a mesh-dependent term controlling the unstable modes of the pressure to the formulation, where this term can depend on residuals of the equation at the element level, or it can just be based on compensating for the inf-sup deficiency of the pressure.

Now, most of the stabilized methods proposed so far rely on the presence of a positive constant multiplying the added term. This constant is called the stabilization parameter, for which a large amount of work has been devoted to looking for the best choice of this parameter, as in some cases the results may heavily depend on it.

In the quest for the best possible parameter, which for us is the one that minimizes the error, we propose to minimize an a posteriori error estimator which will be proved to be fully computable, a rigorous upper bound for the error, and equivalent to the error, with a lower constant independent of the stabilization parameter. Hence, hopefully minimizing this estimator can give us a stabilization parameter which also minimizes the error.

Following this idea, this estimator is built and analysed by *splitting the velocity error* into a conforming and a nonconforming part, which play an important role in the performance. As the finite element space for the velocity is continuous, the so called *equilibrated boundary fluxes* are used to build the estimator in conjunction with the reconstruction of a $\overset{\boldsymbol{H}}{\approx}(\boldsymbol{div},\Omega)$ *conforming lifting*, for which an explicit simple formula can be derived, which allows for some minimization, making the estimation of the velocity error very tight. Finally, the a posteriori error estimator for the pressure follows using the continuous inf-sup condition, and relies on the a priori knowledge of the inf-sup constant. Fortunately, tight estimates for this constant are available in the literature.

Finally, once the estimator is available, we propose the use of a Trust-Region Derivative Free Optimization algorithm to approximate the minimiser of such an estimator with respect to the stabilization parameter.

A posteriori error estimates for linear wave problems

Emmanuil H. Georgoulis, Omar Lakkis & Charalambos Makridakis *(University of Leicester)*

We address the error control of standard discretisations of linear second order hyperbolic problems. More specifically, we derive a posteriori error bounds in various norms for two-step time-stepping methods (drawn from the family of 2nd order cosine schemes) and we discuss the extensions of these results to the fully discrete setting, whereby the space discretisation is based on finite element methods. The derivation of these bounds relies crucially on (classical) ideas for the a-priori error analysis of the same methods due to Baker from the 1970s, as well as on careful constructions of suitable (space-)time-reconstruction functions.

A posteriori error estimates for classical and singularly perturbed parabolic equations

Natalia Kopteva & Torsten Linß *(University of Limerick)*

For classical and singularly perturbed semilinear parabolic equations, we present maximum norm a posteriori error estimates that, in the singulaly perturbed regime, hold uniformly in the small perturbation parameter. The parabolic equations are discretized in time using the backward Euler method, the Crank-Nicolson method and the discontinuous Galerkin dG(1) method. Both semidiscrete (no spatial discretation) and fully discrete cases will be considered. The analysis invokes elliptic reconsturcions and elliptic a posteriori error estimates.

A finite element method for nonlinear elliptic equations

Omar Lakkis & Tristan Pryer *(University of Sussex)*

Fully nonlinear equations are notoriously hard to solve numerically. Finite difference schemes have been known for some of these equations, but the nonvariational structure makes them harder nuts to crack with Galerkin methods. This almost precludes the use of adaptive methods (which come natural for finite element meshes) for the approximate solutions of such equations. In this research we derive a Newton's method to solve fully nonlinear elliptic equations, as well as a fixed point iteration to solve quasilinear equations such as the ∞-Laplacian based on a *nonvariational* Galerkin finite element method. Adaptive methods are derived based on residual-type aposteriori error estimates. Numerical experiments illustrate the derived methods in various situations.

Error estimators for a partially clamped plate problem with bem

Matthias Maischak *(Brunel University)*

The biharmonic equation models the bending of a thin elastic plate. Restricting the corresponding minimization problems on a convex subset of possible boundary conditions describing restrictions on the clamping of the plate boundary, we obtain a variational inequality. Using the fundamental solution we obtain a symmetric integral operator representation. The higher regularity requirements of the biharmonic operator lead to the usage of C^1 basis functions, as well as to a C^1 regular representation of the boundary. We will first present a high-order numerical quadrature scheme, suitable for a hp-method on curved boundaries and second, we will derive a-posteriori error estimates based on a hierarchical decomposition. Several numerical examples underline the theoretical results.

Anisotropic mesh adaptation via a posteriori error estimation

S. Micheletti *(Politecnico di Milano)*

In this communication we present some results concerning the employment of a posteriori error estimation to drive an anisotropic mesh adaptation.

The numerical simulation of advection-diffusion phenomena with strong advection, of the Navier-Stokes equations at large Reynolds number, of ground-water flows in aquifers with varying hydraulic conductivity, where internal and boundary layers may occur - or the unsteady multimaterial simulation of a water column collapsing under gravity, does benefit of the use of an adaptive technique so as to track the space heterogeneities and the time dynamics.

The automatism and reliability of the whole procedure is made possible by the introduction of an a posteriori estimator, or indicator, of the discretization error. In particular, we have developed a posteriori estimates for both the energy norm and linear and nonlinear functionals of the error.

The applications tackled so far comprise standard second-order elliptic problems - diffusion equations and advection dominated advection-diffusion-reaction systems, their parabolic counterpart, as well as the Stokes and Navier-Stokes equations for uncompressible fluids. Recently, we have also dealt with anisotropic mesh adaptation for PDE-constrained optimal control problems.

A residual-based a posteriori estimator for the $\mathbf{A} - \varphi$ magnetodynamic harmonic formulation of the Maxwell system

S. Nicaise, E. Creusé, Z. Tang, Y. Le Menach, N. Nemitz & F. Piriou *(Université de Valenciennes)*

My talk will be devoted to the derivation of an a posteriori residual-based error estimator for the $\mathbf{A} - \varphi$ magnetodynamic harmonic formulation of the Maxwell system. The weak continuous and discrete formulations will be established, and the well-posedness of both of them will be addressed. Some useful analytical tools will be derived; among them, an ad-hoc Helmholtz decomposition will be proven, which allows to pertinently split the error. Consequently, an a posteriori error estimator will be obtained, which will be proven to be reliable and locally efficient. Finally, some numerical tests that confirm the theoretical results will be presented.

A posteriori error estimation for finite element approximations of linear elasticity problems

Richard Rankin & Mark Ainsworth *(University of Strathclyde)*

Finite element approximation schemes can be used to obtain approximate solutions to partial differential equations. When using a numerical method to approximate the solution to any problem it is important to be able to say how accurate the approximation obtained is. We will discuss the a posteriori error estimators that we have obtained for bounding the energy norm of the error in finite element approximations of linear elasticity problems in two and three dimensions.

A posteriori estimates for problems with linear growth energy functionals

Sergey Repin *(Steklov Institute, St Petersburg)*

Energy functionals having linear growth with respect to the norm of the gradient (or strain) operator arise in the theory of nonparametric minimal and capillary surfaces, perfect plasticity, and other problems. Original variational formulations associated with these functionals are incorrect and require a relaxation that leads to problems defined on spaces of functions whose derivatives are Radon measures. The corresponding dual problems are well posed, but defined on rather complicated sets of admissible dual functions. For these reasons, getting fully reliable numerical approximations for such type problems is faced with serious difficulties. In the talk, it is shown a way to construct converging approximations with the help of standard conventional finite element approximations and explicitly control the error with the help of guaranteed a posteriori estimates that has been recently derived for this class of problems.

A posteriori error estimator for the Reissner-Mindlin problem

Emmanuel Verhille, Emmanuel Creusé & Serge Nicaise *(Laboratoire Paul Painlevé)*

We consider the Reissner-Mindlin problem with homogeneous Dirichlet boundary conditions into a domain $\Omega \subset \mathbf{R}^2$ defined by :

$$\begin{cases} -div\, \mathcal{C}\varepsilon(\phi) = \gamma & \text{in } \Omega, \\ -div\, \gamma = g & \text{in } \Omega, \\ \gamma = \lambda t^{-2}(\nabla\omega - \phi) & \text{in } \Omega, \end{cases} \quad (1)$$

where the unknowns are ω, a scalar function which represents the transverse displacement of the median plane of the plate and ϕ, a vector-valued function which represents the rotation of its normal under deformation. t represents the plate thickness, gt^3 the load acting on the plate, $\mathcal{C}$ is the tensor of elastic moduli (depending of the Young modulus and the Poisson coefficient determinated by the plate nature), and λ a Lamé coefficient.

The solution of the problem (1) is approximated by a $\mathbf{P}_1$-conforming finite element method : we look for $(\omega_h, \phi_h) \in \mathbf{P}_1 \times \mathbf{P}_1^2 \subset H_0^1(\Omega) \times H_0^1(\Omega)^2$, that is the approximation of the exact solution (ω, ϕ). The approximation error is defined by

$$e_h^{rot} := \|\omega - \omega_h\|^2_{H_0^1(\Omega)} + \|\phi - \phi_h\|^2_{H_0^1(\Omega)^2} +$$

$$\lambda^{-1}t^2\|\gamma-\gamma_h\|^2_{L^2(\Omega)}+\lambda^{-2}t^4\|rot(\gamma-\gamma_h)\|^2_{L^2(\Omega)}+\|\gamma-\gamma_h\|^2_{H^{-1}(\Omega)}.$$

The aim of this work is to find an a posteriori estimator η, robust on the plate thickness t, totally explicit, leading to an upper-bound of type $e_h^{rot} \leq \eta$ (reliability). We can notice that the multiplicative constant is equal to one in the upper-bound, which constitutes the originality of our work. Our technique is based on the derivation of an equilibrated estimator using two elements named x^* and y^*, totally built from the approximations ω_h and ϕ_h into ad hoc functionnal spaces.
Additionally, we give a lower-bound of type $\eta \leq Ce_h^{rot}$ (efficiency) where the positive constant C depends only on the shape regularity of the mesh. Some numerical tests that confirm the theoretical results will be presented.

A unified framework for a posteriori error estimation for the Stokes problem

Martin Vohralík, A. Hannukainen & R. Stenberg
(Université Paris)

A unified framework for a posteriori error estimation for the Stokes problem is developed. It is based on $[H_0^1(\Omega)]^d$-conforming velocity reconstruction and $[\mathbf{H}(\mathrm{div}, \Omega)]^d$- conforming, locally conservative flux (stress) reconstruction. It gives guaranteed, fully computable global upper bounds as well as local lower bounds on the energy error. In order to apply this framework to a given numerical method, two simple conditions need to be checked. We show how to do this for various conforming and conforming stabilized finite element methods, the discontinuous Galerkin method, the Crouzeix–Raviart nonconforming finite element method, the mixed finite element method, and a general class of finite volume methods. The tools developed and used include a new simple equilibration on dual meshes and the solution of local Poisson-type Neumann problems by the mixed finite element method. Numerical experiments illustrate the theoretical developments.

Minisymposium M2
Practical approximation with polynomials and beyond
Organisers: Pedro Gonnet and Nick Hale

Getting rid of spurious poles: a practical approach

Ricardo Pachón *(Credit Suisse)*

Rational approximation, in theory, is a powerful technique that can overcome deficiencies of polynomial approximation. In practice, however, the use of rational functions is affected by the appearance of spurious poles, also known as "Froissart doublets", artificial pairs of zeros and poles that are introduced in the computed approximation because of rounding errors.

This talk will present work, developed in collaboration with Gonnet, van Deun and Trefethen, for the removal of spurious poles. We have established a connection between them and the singular values of the linear system associated to the rational interpolation problem. Moreover, we have exploited this connection in an algorithm for robust and stable rational approximation, in which the spurious poles are removed and the conditions of the problem are changed from interpolation to least-squares fitting. We will present this strategy in detail as well as many examples.

Approximating functions with endpoint Singularities

Mark Richardson *(University of Oxford)*

In this talk, we describe the 'Sincfun' software system for computing with functions that may have an endpoint singularity. Sincfun is modelled closely on Chebfun, but uses sinc function expansions instead of Chebyshev series. Our experiment sheds light on the strengths and weaknesses of sinc function techniques. It also serves as a review of some of the main features of sinc methods including construction, evaluation, zerofinding, optimization, integration and differentiation.

Convergence theorems for polynomial interpolation in Chebyshev points

Lloyd N. Trefethen *(University of Oxford)*

We present two theorems that quantify the idea that the smoother a function f is, the faster its degree n polynomial interpolants in Chebyshev points converge as $n \to \infty$. The first, going back in essence to Bernstein, asserts convergence at the rate $O(M\rho^{-n})$ if f is analytic with $|f(z)| \leq M$ in the ρ-ellipse around $[-1, 1]$. The second asserts convergence at the rate $O(Vn^{-\nu})$ if f has a νth derivative on $[-1, 1]$ of bounded variation V. Curiously, the latter result does not seem to be in the literature.

Minisymposium M3

Novel algorithms for the solution of boundary-value problems

Organisers: Pedro Gonnet and Nick Hale

Automatic differentiation for automatic solution of nonlinear BVPs

Asgeir Birkisson *(University of Oxford)*

A new solver for nonlinear boundary-value problems (BVPs) in Matlab is presented, based on the Chebfun software system for representing functions and operators automatically as numerical objects. The solver implements Newton's method in function space, where the derivatives involved are Frechet derivatives, computed using automatic differentiation (AD). We present our AD implementation, details of the Newton iteration and show various examples of solving nonlinear BVPs with Chebfun.

Finite difference preconditioners for spectral methods

Pedro Gonnet *(University of Oxford)*

Spectral collocation methods are a powerful tool for the numerical solution of ODEs and systems of ODEs. The solution of a linear ODE in one dimension involves the construction of a dense discretized linear operator L of size $N \times N$, where N is the number of points used to represent the solution. The discretized solution $\underline{u}$ is then computed by solving $L\underline{u} = \underline{f}$ for some right-hand side $\underline{f}$.

Although this solution is straight-forward and relatively easy to implement for single equation or systems of equations, it involves solving for the dense matrix L, which typically requires $\mathcal{O}(N^3)$ operations, making this method prohibitively expensive for large N or large systems.

An alternative going back to Orszag (1980) and studied extensively by Canuto and Quarteroni (1985) and Funaro (1987) is to solve the linear system of equations $L\underline{u} = \underline{f}$ iteratively using preconditioned GMRES. As a preconditioner, a finite difference approximation of the operator can be used, which is sparse and easily invertible. Evaluating the operator does not require forming the matrix L and can be done in $\mathcal{O}(N \log N)$ operations. This reduces the total cost of solving the linear system of equations from $\mathcal{O}(N^3)$ to $\mathcal{O}(N \log N)$.

In this talk, we discuss efficient ways of constructing and applying this preconditioner, some results on its performance and general applicability, as well as the implementation of this solver as part of the Chebfun system.

"Rectangular pseudospectral differentiation matrices" or, "Why it's not hip to be square"

Nick Hale & Toby Driscoll *(University of Oxford)*

The standard way of including boundary conditions in spectral collocation methods involves replacing certain rows of the matrices with others that enforce the required conditions. For example, in a two-point boundary value problem with Dirichlet conditions at each end, one replaces the first and last rows with `[1,zeros(1,N-1)]` and `[zeros(1,N-1),1]` respectively. However, a few things are troublesome with this kind of approach:

- for more general boundary conditions the choice of which rows to replace is often heuristic,
- the wrong choice can lead to singular matrices (particularly in systems of equations),
- interpolation at just interior Chebyshev nodes can have a much larger Lebesgue constant,
- products of differentiation and integration matrices do not produce the identity matrix.

In this talk we discuss an alternative approach, whereby the collocation matrix is projected onto a lower degree subspace to make it rectangular and the boundary conditions used to 'square it up'. We show how this approach can be implemented by a simple pre-processing step, and demonstrate that it overcomes the difficulties mentioned above. We explore connections with other ideas in the literature, such as the use of staggered grids and the 'fictitious points' advocated by Fornberg, and finally we show the rectangular matrices in action on some boundary value and eigenvalue problems.

Minisymposium M4

Stochastic computation

Organisers: Evelyn Buckwar and Des Higham

Multi-level Monte Carlo Finite Element methods for elliptic PDEs with stochastic coefficients

Andrea Barth *(University of Zurich)*

In Monte Carlo methods quadrupling the sample size halves the error. In simulations of stochastic partial differential equations (SPDEs), the total work is the sample size times the solution cost of an instance of the partial differential equation. A Multi-Level Monte Carlo method is introduced which allows, in certain cases, to reduce the overall work to that of the discretization of one instance of the deterministic PDE. The model problem is an elliptic equation with stochastic coefficients. Multi-Level Monte Carlo errors and work estimates are given both for the mean of the solutions and for higher moments. The overall complexity of computing mean fields as well as as k-point correlations of the random solution is proved to be of log-linear complexity in the number of unknowns of a single Multi–Level

solve of the deterministic elliptic problem. Numerical examples complete the theoretical analysis.

Linear Stability Analysis of Numerical Methods for Stochastic Differential Equations

Evelyn Buckwar, Cónall Kelly & Thorsten Sickenberger *(Heriot-Watt University)*

Stochastic differential equations are increasingly used in several application areas to model random dynamics, the influence of physical noise or uncertainties in system parameters. Numerical methods are a necessary tool to study the mathematical models and thus in recent years stochastic numerics has made considerable progress. In this talk I will provide an overview of available methods and results for a linear stability analysis of numerical methods for systems of stochastic differential equations.

From cells to tissue: coping with the heterogeneity via fractional models

Kevin Burrage, Nicholas Hale and David Kay *(University of Oxford)*

Fractional differential equations are becoming increasingly used as a modelling tool for coping with anomalous diffusing processes and heterogeneous media. However, the presence of a fractional differential operator causes memory (time fractional) or nonlocality (space fractional) issues and this imposes a number of computational constraints. In this talk we discuss how fractional equations arise from stochastic processes with heavy tails and then develop efficient, scalable techniques for solving fractional-in-space reaction diffusion equations using the finite element method and robust techniques for computing the fractional power of a matrix times a vector. Our approach is show-cased by solving the fractional Fisher and fractional Allen-Cahn reaction-diffusion equations in two spatial dimensions and analysing the speed of the travelling wave and size of the interface in terms of the fractional power of the underlying Laplacian operator.

Using a modification of the SSA to simulate spatial aspects of chemical kinetics

Pamela Burrage, Tamas Szekely & Kevin Burrage *(Queensland University of Technology)*

It is now well recognised that the dynamics of chemical kinetics, when there are small numbers of interacting particles, is best described by the Stochastic Simulation Algorithm (SSA). It is also recognised that in some cases, spatial variants are needed when there are spatial heterogeneities or spatial confinements. However, such implementations can be extremely computationally intensive.

In this talk we present a model of the colorectal crypt where there is a small niche of stem cells that differentiate into other types of cells, which then migrate through the crypt. Our approach is to introduce a probability density function representing the time for a cell to be absorbed at the ends of the crypt, and this allows us to modify the SSA by using this important spatial information without actually performing a detailed Monte Carlo simulation. We attempt to estimate the accuracy and efficiency of this approach.

Numerics for quadratic FBSDE

Gonçalo Dos Reis *(TU Berlin)*

In this presentation we discuss a class of stochastic differential equations (SDE) named Forward-Backward SDE (FBSDE) and give particular attention to the so-called quadratic case. We explain how this class links to semilinear Partial differential equations (PDE) with quadratic non linearity in the gradient component. We cover some of the main results and difficulties concerning the numerics for quadratic FBSDE.

Optimal Error Estimates of Galerkin Finite Element Methods for SPDEs with Multiplicative Noise

Raphael Kruse *(University of Bielefeld)*

In this talk we focus on Galerkin finite element methods for semilinear stochastic partial differential equations (SPDEs) with multiplicative noise and Lipschitz continuous nonlinearities. We analyze the strong error of convergence for spatially semidiscrete approximations as well as a spatio-temporal discretization which is based on a linear implicit Euler-Maruyama method. In both cases we obtain optimal error estimates. The results hold for different Galerkin methods such as the standard finite element method or spectral Galerkin approximations.

If time permits we give a sketch of the proofs which are based on sharp integral versions of well-known error estimates for the corresponding deterministic linear homogeneous equation together with optimal regularity results for the mild solution of the SPDE.

Lax's equivalence theorem for stochastic differential equations

Annika Lang *(University of Zurich)*

Lax's equivalence theorem is a well-known result in the approximation theory of partial differential equations. It states: If an approximation is consistent, stability and convergence are equivalent. In this talk I will generalize this result to Hilbert space valued stochastic differential equations. Furthermore, examples will illustrate consistency, stability, and convergence for some approximations of Hilbert space valued stochastic dfferential equations.

Euler–Maruyama-type Numerical Methods for Stochastic Lotka-Volterra Model

Wei Liu & Xuerong Mao *(University of Strathclyde)*

Consider the one-dimensional stochastic Lotka-Volterra model

$$dx(t) = (bx(t) - ax^2(t))dt + \sigma x(t)dB(t), \qquad (2)$$

with positive parameters a, b and σ. Many authors have investigated this stochastic population model, from its explicit solution through extinction to stationary distribution. These theoretical results form an excellent base to test the ability of numerical methods for highly non-linear stochastic differential equations (SDEs).

In this talk, we are concerned with the Euler–Maruyama-type numerical methods. It is known that given a positive initial value $x(0)$ at $t = 0$, the stochastic Lotka-Volterra model has a unique global positive solution $x(t)$ on $t \in [0, \infty)$. However this is not the case for the explicit Euler-Maruyama (EM) method

$$X_{k+1} = X_k + (bX_k - aX_k^2)\Delta t + \sigma X_k \Delta B_k, \qquad (3)$$

due to the unboundedness of the normally distributed Brownian increment $\Delta B_k := B((k+1)\Delta) - B(k\Delta)$. To preserve the positivity of the EM method, we introduce the stopped EM approximate solution using the technique of stopping time. The existing known results have only so far shown that the stopped EM approximate solution converges to the true solution in probability. One of our key contributions here is to show that it converges to the true solution in the strong sense (namely L^2).

Moreover, the underlying SDE (2) is almost surely exponentially stable if $b - (1/2)\sigma^2 < 0$. We have not been able to show that the stopped EM method is almost surely exponentially stable under this same condition for sufficiently small step-size Δt. However, we introduce a weak backward EM method and successfully show that it reproduces this stability property.

Numerical Simulation of Stochastic Reaction Networks modelled by Piecewise Deterministic Markov Processes

Martin Riedler *(Heriot-Watt University)*

Hybrid systems, and Piecewise Deterministic Markov Processes in particular, are widely used to model and numerically study multiscale systems in biochemical reaction kinetics and related areas where I put an emphasise on models arising in mathematical neuroscience. I will present an almost sure convergence analysis for numerical simulation algorithms for Piecewise Deterministic Markov Processes. These algorithm are built by appropriately discretising constructive methods defining these processes. The stochastic problem of simulating the random, path-dependent jump times is reformulated as a hitting time problem for a system of ordinary differential equations with random threshold which is solved using continuous approximation methods. In particular show that the almost sure asymptotic convergence rate of the stochastic algorithm is identical to the order of the embedded deterministic method. Finally, we present an extension of our results to more general Piecewise Deterministic Processes.

Mean Exit Times and Multi-Level Monte Carlo Simulations

Mikolaj Roj, Des Higham, Xuerong Mao, Qingshuo Song & George Yin *(University of Strathclyde)*

Many financial quantities such as path dependent options, volatility swaps and credit risk models are based on simulations of stopping times. One has to use Monte Carlo simulations especially when a high number of dimensions is involved. However, numerical methods for stochastic differential equations are relatively inefficient when used to approximate mean exit times. In particular, although the basic Euler–Maruyama method has weak order equal to one for approximating the expected value of the solution, the order reduces to one half when it is used in a straightforward manner to approximate the mean value of a (stopped) exit time. Consequently, the widely used standard approach of combining an Euler-Maruyama discretization with a Monte Carlo simulation leads to a computationally expensive procedure. In this work, we show that the multi-level approach developed by Giles (Operations Research, 2008) can be adapted to the mean exit time context. In order to justify the algorithm, we analyse the strong error of the discretization method in terms of its ability to approximate the exit time. We then show that the resulting multi-level algorithm improves the expected computational complexity by an order of magnitude, in terms of the required accuracy. Computational results are provided to illustrate the analysis.

Efficient Multilevel Monte Carlo simulations of nonlinear financial SDEs without a need of simulating Levy areas.

Lukasz Szpruch *(University of Oxford)*

In many financial engineering applications, one is interested in the expected value of a financial derivative whose payoff depends upon the solution of a stochastic differential equation. Using a simple Monte Carlo method with a numerical discretization with first order weak convergence, to achieve a root-mean-square error of $O(\epsilon)$ would require $O(\epsilon^{-2})$ independent paths, each with $O(\epsilon^{-1})$ time steps, giving a computational complexity which is $O(\epsilon^{-3})$. Recently, Giles [Giles, 2008] introduced a Multilevel Monte Carlo (MLMC) estimator, which enables a reduction of this computational cost to $O(\epsilon^{-2})$. In order to achieve this superior property of the MLMC estimator, the numerical discretization of a SDEs under consideration requires certain convergence properties, namely that the numerical approximation strongly converge to the solution of the SDEs with order 1. This carries some difficulties. First of all, it is well known that it impossible to obtain an order of convergence higher than 0.5 without a good approximation of the Levy areas (which are very expensive to simulate) [Cameron, 1980]. Second, convergence and stability

of numerical methods are well understood for SDEs with Lipschitz continuous coefficients, whereas most financial SDEs violates these conditions. It was demonstrated, that for SDEs with non-Lipschitz coefficients using the classical methods, we may fail to obtain numerically computed paths that are accurate for small step-sizes, or to obtain qualitative information about the behaviour of numerical methods over long time intervals [Jentzen, 2011]. Our work addresses both of these issues, giving a customized analysis of the most widely used numerical methods. In this work we generalize the current theory of strong convergence rates for Euler-Maruyama-type schemes for some highly non-linear multidimensional SDEs which appear in finance. We also construct a new MLMC estimator that enables us to avoid simulation of Levy areas without affecting the required computational cost of order $O(\epsilon^{-2})$. We support our theoretical results with the simulations of expected values of options with various payoffs.

Adaptive stepsize control for the strong numerical solution of SDEs

Phillip Taylor *(University of Manchester)*

The strong numerical solutions of stochastic differential equations (SDEs) can be found using numerical methods such as the Euler-Maruyama method and the Milstein method. The use of fixed stepsizes for these methods has been widely studied; however the theory for using adaptive stepsize control is far less developed, and there are many issues to consider. Firstly, we must be careful since there are methods which may look sensible but converge to the wrong solution. Once we have a method which converges to the right solution we have, for example, many choices of error estimates at each step, and different choices for how we can change the stepsize and generate the Wiener path. Some methods may be suitable for solving SDEs generated by a one-dimensional Wiener process but less suitable if the Wiener process is multi-dimensional. We investigate different approaches to solving both Ito and Stratonovich SDEs using adaptive stepsize control, and the issues involved.

Minisymposium M5

Iterative linear solvers for PDEs

Organiser: Andy Wathen

Fast Multigrid Algorithms and High Order Variational Image Registration Model

Ke Chen *(University of Liverpool)*

Variational partial differential equations (PDEs) based methods can be used for deformable image registration to derive reliable results for many cases Modersitzki [1]. One challenge inherent from other regularization modeling such as denoising is that it is not trivial to design a single model suitable for both smooth and non-smooth deformation problems. A model based on a curvature type regularizer [2-3] appears to deliver excellent results for both problems and is proposed and studied in this paper. We address the problem of developing a fast algorithm for the system of two coupled PDEs which is highly nonlinear and of fourth order.

In this paper, we first study several fixed-point type smoothers, their local Fourier analysis and experiments to select the most effective smoother before using a nonlinear multigrid algorithm for the new model. We then generalize the work to multi-modal image registration modeling based on combining intensity and geometric transformations. Numerical tests showing advantages of our new models and algorithms are given.

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Interface Preconditioners for Flow Problems

Daniel Loghin *(University of Birmingham)*

Domain decomposition methods are established techniques for solving linear systems arising from the discretization of PDE. A key feature of these methods is the solution of the interface problem (or interface Schur complement) arising from a non-overlapping decomposition of the domain. For certain scalar PDE (e.g., elliptic problems) the fast resolution of this problem is possible through a range of robust algorithms. However, the generalization of these methods to the case of systems of PDE is not always straightforward.

In this talk we examine a class of interface preconditioners for the Stokes and the Oseen and Navier-Stokes equations. The analysis considers the continuous interface problem and its discrete counterpart under various standard mixed finite element discretizations of the full problem. We show that the coercivity and continuity of the bilinear forms induced by the interface operator provide mesh-independent preconditioners for both the Stokes and Oseen problems. For the Navier-Stokes system, we indicate how additional adaptive preconditioning techniques can be used to enhance performance. Numerical results using standard test problems are included to illustrate the procedure and verify the optimality of the proposed solver technique.

Sharp performance estimates for optimized domain decomposition preconditioners

Sébastien Loisel & Stephen W. Drury *(Heriot-Watt University)*

The numerical solution of elliptic boundary value problems is important in many fields of applications. Domain decomposition methods can be used to solve such problems in parallel on supercomputers. Optimized domain decomposition methods introduce a "Robin parameter" which can be tuned for higher performance. The analysis of such methods has been very challenging. In this talk, we will discuss symmetric and nonsymmetric optimized domain decomposition methods and we will give new performance estimates for the nonsymmetric methods used in combination with the GMRES algorithm.

Preconditioned Iterative Methods for Convection-Diffusion Control Problems

John Pearson & Andrew J. Wathen *(University of Oxford)*

The development of iterative solvers for solving linearized systems of equations arising from finite element discretizations of partial differential equations (PDEs) is a well-established field of numerical analysis. A more recent area of interest is finding solvers for optimization problems with PDE constraints, so called PDE constrained optimization problems. We consider a particular class of problems of this type, namely distributed convection-diffusion control problems. Using an appropriate stabilization technique, the Local Projection Stabilization method, we develop preconditioned MINRES and Bramble-Pasciak Conjugate Gradient solvers for such problems. To create these solvers, we draw on ideas from saddle point theory, the approximation of finite element mass matrices, and multigrid techniques for the solution of convection-diffusion operators. We present supporting theory and numerical results to demonstrate the effectiveness and scope of our iterative methods.

Saddle-point Problems in Liquid Crystal Modelling

Alison Ramage and Chris Newton *(University of Strathclyde)*

The focus of this work is on the iterative solution of saddle-point problems which occur frequently, and in multiple ways, in liquid crystal numerical modelling. For example, saddle-point problems arise whenever director models are implemented, through the use of Lagrange multipliers for the pointwise unit vector constraints (as opposed to using angle representations). In addition, saddle-point systems arise when an electric field is present that stems from a constant voltage, irrespective of whether a director model or a tensor model is used, or whether angle representations for directors or componentwise representation with pointwise unit vector constraints is employed. Furthermore, the combination of these two situations (that is, a director model using components, associated constraints and Lagrange multipliers, together with a coupled electric field interaction) results in a novel double/inner saddle-point structure which presents a particular challenge in terms of numerical linear algebra.

In this talk we will present some examples of the saddle-point systems which arise in liquid crystal modelling and discuss their efficient solution using appropriate preconditioned iterative methods with the aim of giving an insight into this new and exciting research area at the interface between liquid crystal theory and numerical analysis.

Fast Iterative Solvers for Saddle Point Problems

David Silvester *(University of Manchester)*

We discuss the design of efficient numerical methods for solving symmetric indefinite linear systems arising from mixed approximation of elliptic PDE problems with associated constraints. The novel feature of our iterative solution approach is the incorporation of error control in the natural energy norm in combination with an 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. We describe a proof of concept MATLAB implementation of this algorithm, which we call EST MINRES, and we illustrate its effectiveness when integrated into our Incompressible Flow Iterative Solution Software (IFISS) package (available online from http://www.manchester.ac.uk/ifiss/). This is joint work with Valeria Simoncini.

Minisymposium M6

Complex Networks and Matrix Computations

Organisers: Des Higham and Alastair Spence

Googling the brain: Discovering hierarchical and asymmetric structure, with applications in neuroscience

Jonathan J. Crofts and Desmond J. Higham *(Nottingham Trent University)*

Hierarchical organization is a common feature of many directed networks arising in nature and technology. As an example, a well-defined message-passing framework based on managerial status typically exists in a business organisation. However, in many real-world networks such patterns of hierarchy are unlikely to be quite so transparent. Due to the nature with which empirical data is collated the nodes will typically be ordered so as to obscure any underlying structure, in addition to this, the presence of a small number of links violating the so-called "chain of

command" makes the determination of such structures extremely challenging. Here we address the issue of how to reorder a directed network in order to reveal this type of hierarchy. Using ideas from the graph Laplacian literature, we show that a relevant discrete optimization problem leads to a natural hierarchical node ranking. In addition, we present a generalisation of this node ordering algorithm based upon the combinatorics of directed walks and show that there exists a natural link between the ideas presented here and Google's PageRank algorithm. We finish by showing how the algorithms perform when applied to both synthetic networks and a real-world network from neuroscience where results may be validated biologically.

Bistability Through Triad Closure

Desmond J. Higham, Peter Grindrod & Mark C. Parsons *(University of Strathclyde)*

The digital revolution is generating novel large scale examples of connectivity patterns that change over time. This scenario may be formalized as a graph with a fixed set of nodes whose edges switch on and off. For example, we may have networks of interacting mobile phone users, emailers, on-line chat room participants, Facebookers or Tweeters. To model and simulate the key properties of such evolving networks, we can use a discrete time Markov chain setting, where edges appear and disappear according to appropriate probabilistic laws. I will describe a new model based on a natural 'triad closure' mechanism that quantifies effects observed in social network analysis—new friendships are more likely between individuals who share current friends. A mean field analysis for this type of evolution leads to a bistable difference equation—the system can evolve into one of two possible steady states. Predictions from the analysis will be illustrated with computational simulations. I will also look at the issue of calibrating the model to a real set of telecommunications data.

Bipartite Subgraphs and the Signless Laplacian Matrix

Steve Kirkland & Debdas Paul *(National University of Ireland Maynooth)*

Motivated by a problem arising in protein-protein interaction networks, we consider the use of the so-called signless Laplacian matrix to help identify bipartite induced subgraphs of a given graph. Specifically, we use the eigenvectors of the signless Laplacian matrix corresponding to small eigenvalues in order to help find bipartite induced subgraphs. We present some theoretical results that help to justify the approach, and apply the technique to a particular protein-protein interaction network.

Reordering multiple networks

Clare Lee, Desmond J. Higham, J. Keith Vass & Daniel Crowther *(University of Strathclyde)*

Many large, complex networks contain hidden substructures that can be revealed using a range of post-processing algorithms. In particular, reordering network nodes appropriately may help to summarise key properties by exposing significant clusters, or more generally sets of neighbours with similar features. Our results have been tested on real data concerning the behaviour of genes and proteins in cells. Microarray data produces large non square matrices of information recording the behaviour of a large number of genes across a small number of samples. This data is by its very nature non-negative. One aim is to cluster or order the genes/samples into groups where members behave similarly to each other and differently to those in other groups. This allows us to find sets of genes whose behaviour distinguishes different sample types. This work focuses on the use of matrix factorisation methods to derive useful network reordering. These methods typically factorise the original matrix into two smaller matrices with a pre-specified number of rows/columns. In particular we look at non-negative matrix factorization techniques, which have the intuitive advantage of respecting the non-negative nature of the original data. We have also developed a non-negative matrix factorisation technique that reorders multiple data sets simultaneously. This has allowing us to incorporate multiple measurements of a similar type as well as other types of information.

Networks in Neuroscience: Using the Generalised Singular Value Decomposition to Compare Pairs of Networks

M McDonald, Des Higham, Neil Dawson & Judy Pratt *(University of Strathclyde)*

In this talk, we will look at a pair of graphs and discuss a problem of comparison, with a view to identifying and examining clustering, eventually also making account of known relationships between different groups of nodes. We describe the use the Generalised Singular Value Decomposition (GSVD) - a close relative of Principal Component Analysis (PCA) to re-order the data such that the clustering is seen.

We will show that, by design, this compares both graphs at the same time, identifying structures that are mutually exclusive to each. Finally, an example where the algorithm is applied to neuroscience data is provided - here the the graphs represent activity in the brain of control and drug dosed rats. We calculate the variance of sub-groups of brain regions within the re-ordered data and propose that this represents the expression of those groups of nodes. Using this approach, we identified structures that are consistent with current biological understanding and suggestive of other areas for examination.

Dynamic Communicators

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

With new technologies and applications a plethora of data sets with novel properties have emerged. We look at data sets which are produced by snap shots of networks over

time. Most methods of analysis have been done assuming a static network. To demonstrate and reinforce methodology for analysing temporal networks, we develop a model with a property observed in voice mail, email, and intuitively plausible for organisations.
Dynamic communicators have an in uence that is hidden when an aggregate view of the time course of a network is viewed. The model is able to create these dynamic communicators in the messages exchanged between them over the time course of the simulations. A key feature is that there is a representation of hierarchy amongst nodes which affects the temporal downstream message propagation. Computational tests on the synthetically produced data reveal this feature.

Temporal Graphs and Robustness

Mirco Musolesi & Vito Latora *(University of St Andrews)*

The analysis of social and technological networks has attracted a considerable attention as social networking applications and mobile sensing devices have given us a wealth of real data about people interactions. Classic studies looked at analysing static or aggregated networks, i.e., networks that do not change over time or built as the result of aggregation of information over a certain period of time. Given the soaring number of collections of measurements related to very large real network traces, researchers are quickly starting to realise that connections are inherently varying over time and exhibit more dimensionality than static analysis can capture.

We have recently proposed a novel theoretical framework to study this class of networks in order to quantify for example the speed/delay of information diffusion processes and structural properties, such as the presence of connected components. We have showed how these metrics are able to capture the temporal characteristics of time-varying graphs, such as delay, duration and time order of interactions, compared to the metrics used in the past on static graphs.

A key aspect is network robustness: the problem we are facing in characterising it is related to the fact that most of the classic definitions of centrality, considering both static and temporal graphs, are based on *shortest* paths. By using these metrics, alternative paths (or walks) are not taken into consideration. However, among the existing definitions of centrality for static graphs, there are some metrics that are calculated considering *all existing* walks; the most used are probably the so-called *Bonacich* and *Katz centrality*. Therefore, a possible solution is to derive a measure of centrality based on multiple paths for temporal graphs. An alternative is to try to "transform" a temporal graph into a static graph and then apply the definitions and use the theoretical results obtained for static graphs. In order to do so, we introduce the concept of reachability graphs as a way of *projecting* temporal graphs into static graphs.

In this talk I will give a brief overview of the proposed conceptual framework and I will present some initial ideas about the calculation of centrality metrics for characterising network robustness by means of matrix computations using the transformation of temporal graphs into reachability graphs.

A graph model to explain the origin of early proteins

Chanpen Phokaew, D. Higham & E. Estrada *(University of Strathclyde)*

We propose and analyse a mathematical model which describes the evolutionary process of residue networks in a prebiotic condition. The model iteratively generates the connectivity structure. We have conducted computational experiments to compare this model with real protein residue networks based on various network properties, including average pathlength, degree distribution and assortativity coefficient. We illustrate that after a relaxation process, our artificial residue networks have network properties that match real protein residue networks.

Communicability of networks

Zhivkho Stoyanov *(University of Bath)*

In this talk we shall discuss the notion of communicability of networks, which evolve with time. In particular, for each agent in the network we shall consider two quantities: the amount of information which passes from, and through, that agent. We shall show that these two quantities can be derived as a result of asymmetry in a matrix associated with the network; this matrix will be called the communicability matrix of the network. A reason for the asymmetry in the communicability matrix is the order in which a sequence of events takes place on the network. We shall conclude the talk by discussing a way of quantifying the significance of a given sequence of events.

Minisymposium M7

Numerical methods for singularly perturbed problems

Organisers: Natalia Kopteva and Martin Stynes

Stabilization of convection-diffussion problems by Shishkin mesh simulation

Bosco Garcia-Archilla *(Univerisdad de Sevilla)*

Standard numerical methods are liable to perform poorly in convection-diffusion problems, particularly on convection-dominated situations, where spurious (unphysical oscillations) are likely to pollute the numerical approximation. Several techniques have been developed in the past 30 years to flatten the unwanted oscillations, although no clear winner has turned up yet. Among the most successful ones are the use of Shishkin meshes, their disadvantage being the difficulty of designing them on nontrivial geome-

tries. We present a technique to simulate Shishkin meshes without the need to build them. The technique is applicable to irregular grids and on nontrivial geometries. The numerical approximation obtained present similar accuracy and lack of oscillations as real (not simulated) Shishkin meshes.

Time and space–accurate numerical solution of one-dimensional parabolic singularly perturbed problems of reaction–diffusion type

José Luis Gracia & C. Clavero *(Universidad de Zaragoza)*

In this talk we consider a parabolic singularly perturbed problem given by

$$\begin{cases} u_t + L_{x,\varepsilon}u = f(x,t), \quad (x,t) \in Q = (0,1)\times(0,T], \\ u(x,0) = 0,\ x \in \overline{\Omega},\ u(0,t) = u(1,t) = 0,\ t \in (0,T], \end{cases} \tag{4}$$

where the spatial differential operator $L_{x,\varepsilon}$ is defined by $L_{x,\varepsilon}u \equiv -\varepsilon u_{xx} + b(x,t)u$. We assume that the singular perturbation parameter satisfies $0 < \varepsilon \leq 1$ and it can be arbitrarily small, and also that sufficient compatibility and regularity conditions hold among the data of the problem. It is well known that, in general, the solution has a multiscale character, which exhibits strong gradients in narrow regions (boundary layers) close to both edges $x = 0$ and $x = 1$, of width $O(\sqrt{\varepsilon}|\ln\varepsilon|)$.

The aim of this talk is twofold: to construct a robust scheme, with respect to the singular perturbation parameter, and that the numerical method has high order convergence in the maximum norm. This norm is the most appropriate in the context of singular perturbation problems, since the maximum error occurs in the boundary layer regions, but it makes more difficult the analysis of the convergence. In this talk the analysis of the convergence is based on two steps: first a semidiscretization in time and afterwards the resulting semidiscrete problems are discretized in space. In this way the analysis of the convergence of the fully discrete scheme is eluded.

In time we discretize by using the backward Euler method on a uniform mesh, and in space we consider a hybrid fourth order compact finite difference scheme of positive type, which is constructed on a special nonuniform mesh condensing the grid points in the boundary layer regions. The discrete maximum principle at each time level can be applied in the analysis based on the two step discretization technique, which does not hold if the fully discrete scheme is considered instead of our approach. To deduce appropriate bounds of the error, we will need to know the asymptotic behavior, with respect to ε, of the solution of the semidiscrete problems at each time level and its derivatives, showing the dependence on the singular perturbation parameter. These bounds can be obtained using an inductive argument. Then, a robust numerical method, having first order in time and almost four order in space in the maximum norm, can be theoretical analyzed.

On the other hand, to increase the order of uniform convergence in time of the fully discrete method it is a difficult task. So, in the second part of this talk, we will show the theoretical difficulties appearing in the analysis of the uniform convergence when the Crank–Nicolson method is used in the time discretization instead of the backward Euler method. To finish, we propose the Richardson extrapolation as an alternative to increase the global order of uniform convergence of the numerical scheme, showing in practice the efficiency of this technique. This research was partially supported by the project MEC/FEDER MTM 2010-16917 and the Diputación General de Aragón.

Collocation methods for singularly perturbed reaction-diffusion equations

Torsten Linß, Goran Radojev & Helena Zarin *(Universität Duisburg-Essen)*

A reaction-diffusion equation in one dimension is discretised by collocation using piecewise quadratic C^1-splines. The method is shown to be robust with respect to the diffusion parameter on a modified Shishkin mesh. The rate of uniform convergence in the maximum norm is almost two. A posteriori error estimates are also derived. These allow the design of an adaptive mesh algorithm. Numerical results illustrate the theoretical findings.
This work is supported by Deutscher Akademischer Austauschdienst; Grant 50740187.

Supercloseness of the SDFEM for convection-diffusion problems with reduced regularity

Lars Ludwig *(Technical University of Dresden)*

The streamline-diffusion finite element method (SDFEM) is applied to a convection-diffusion prob- lem posed on the unit square using a rectangular mesh and bilinear elements. With u being the exact solution, the usual error estimates for $\| u^I - u_h \|_{SD}$ require a regularity of at least $u \in H^3(\Omega)$.). In many cases, e.g. for polygonal domains or non-smooth data, this regularity cannot be taken for granted. It will be shown that supercloseness results still hold in some sense if the exact solution has reduced regularity. Finally, numerical experiments illustrate the theoretical findings

A Linear Singularly Perturbed Problem with an Interior Turning Point

J. Quinn *(Dublin City Univerity)*

In this talk we examine the linear singularly perturbed problem: Find y_ϵ such that

$$L_\epsilon y_\epsilon(x) := (\epsilon y_\epsilon'' - a_\epsilon y_\epsilon' - b y_\epsilon)(x) = f(x), \quad x \in \Omega := (0,1), \tag{5a}$$

$$y_\epsilon(0) = A > 0, \quad y_\epsilon(1) = B < 0, \quad b(x) \geq 0, x \in \Omega, \tag{5b}$$

$$d \in \Omega: \quad a_\epsilon(x) \geq 0, x \in [0,d), \quad a_\epsilon(d) = 0, \tag{5c}$$

$$a_\epsilon(x) \leq 0, x \in (d,1], \tag{5d}$$

$$|a_\epsilon(x)| \geq |\alpha_\epsilon(x)|, \quad x \in \Omega, \tag{5e}$$

$$\alpha_\epsilon(x) := \theta \tanh\Big(\frac{r}{\epsilon}(d-x)\Big), \theta, r > 0. \tag{5f}$$

The numerical analysis for this problem differs from the standard analysis for a problem with a non-zero discontinuous convective coefficient of the form $a > 0, x < d,\ a < 0, x > d$. Existence of a solution is first established across Ω, before the analysis for problem is split at the point where the coefficient a_ϵ becomes zero. An upwind finite difference operator is combined with a piecewise-uniform Shishkin mesh centered around d to generate numerical approximations. Numerical results are presented to illustrate the theoretical parameter-uniform error bounds established. This research is funded by the Irish Research Council for Science, Engineering and Technology.

A balanced finite element method for singularly perturbed reaction-diffusion problems

Martin Stynes & Runchang Lin *(National University of Ireland, Cork)*

Consider the singularly perturbed linear reaction-diffusion problem $-\varepsilon^2\Delta u + bu = f$ in $\Omega \subset R^d$, $u = 0$ on $\partial\Omega$, where $d \geq 1$, the domain Ω is bounded with (when $d \geq 2$) Lipschitz-continuous boundary $\partial\Omega$, and the parameter ε satisfies $0 < \varepsilon \ll 1$. It is argued that for this type of problem, the standard energy norm $[\varepsilon^2|u|_1^2 + \|u\|_0^2]^{1/2}$ is too weak a norm to measure adequately the errors in solutions computed by finite element methods because the multiplier ε^2 gives an unbalanced norm whose different components have different orders of magnitude. A balanced and stronger norm is introduced, then for $d \geq 2$ a mixed finite element method is constructed whose solution is quasi-optimal in this new norm. By a duality argument it is shown that this solution attains a higher order of convergence in the L_2 norm. Error bounds derived from these analyses are presented for the cases $d = 2, 3$. For a problem posed on the unit square in R^2, an error bound that is uniform in ε is proved when the new method is implemented on a Shishkin mesh. Numerical results are presented to show the superiority of the new method over the standard mixed finite element method on the same mesh for this singularly perturbed problem.

Minisymposium M8

Recent Advances in Numerical Linear Algebra

Organiser: Françoise Tisseur

Two Two-Sided Procrustes Problems Arising in Atomic Chemistry

Rüdiger Borsdorf *(University of Manchester)*

In atomic chemistry it is of interest to obtain a minimal set of localized atomic orbitals that describes the atom of interest and ensures certain properties of the atom. The set is to be obtained from a density operator of a molecular system with large dimensions computed from results in quantum chemistry.

Let $N \in \mathbb{R}^{n\times n}$ be symmetric and represent the density operator. Let $D \in \mathbb{R}^{m\times m}$ with $m < n$ be given and diagonal. The first problem that we are looking at is to minimize $\|Y^TNY - D\|_F^2$ over $Y \in \mathbb{R}^{n\times m}$ having orthonormal columns and with $\|\cdot\|_F$ denoting the Frobenius norm. This problem is equivalent to finding a minimal set describing an atom with occupation numbers closest to the prescribed diagonal elements of D. In the second problem only the number of electrons in the atom is desired to be close to a prescribed value $d \in \mathbb{Z}$, which is equivalent to minimizing the objective function $(\text{trace}(Y^TNY) - d)^2$. Both optimization problems involve the minimization over the Stiefel manifold and are of the form of the two-sided Procrustes problem.

Looking at the stationary points of the first problem on the manifold reveals the equivalence of this problem to an imbedding problem. This allows the application of a theorem by Fan and Pall from 1957 yielding the minimum function value. From this result we also obtain an optimal solution. By means of this analysis we show the equivalence of the second problem to a convex quadratic problem with box constraints. To solve this problem we propose to use the active-set method, as an optimal solution of the inner optimization problem can easily be obtained. Hence, this method yields a solution at low computational cost.

Blocked Methods for Computing the Square Root of a Matrix

Edvin Deadman *(University of Manchester)*

The square root of a matrix can be computed via a Schur decomposition. The square root of the resulting triangular matrix can then be found either a column at a time or a superdiagonal at a time. However this method does not take advantage of level 3 BLAS operations. In this talk I will discuss implementations of the Schur method which use blocking and recursion to enable the square root to be computed using level 3 BLAS. I will describe the speedups obtained and will discuss applications to other triangular matrix computations.

A Linear Algebraist's Approach to Reforming The UK Voting System

Philip A. Knight *(University of Strathclyde)*

Many modern democracies use forms of proportional representation (PR) as a means of allocating members of parliament at both local and national level. The UK has joined in recently and a number of elections (e.g., European, Scottish) use forms of PR; although there is strong resistance to bringing it into the Westminister election, as the recent vote on AV indicates.

Biproportional apportionment is a novel method of applying PR, used for the first time in 2006 in Switzerland. It works by applying a discrete form of matrix balancing. We investigate the viability of biproportional assignment in UK elections; in particular how to overcome its limitations when applied to a system with over 600 constituencies all requiring a single representative. We show that

a new multi-level apportionment process can be applied, but also look at alternative approach based on optimising network flow. We discuss pros and cons of such a system.

Along the way we prove a new convergence result for matrix balancing.

A method for the computation of Jordan blocks in parameter-dependent matrices

Alastair Spence *(University of Bath)*

Preconditioning for GMRES

Andy Wathen & Jen Pestana *(University of Oxford)*

For linear systems of equations with a real symmetric (or complex hermitian) coefficient matrix, there are standard iterative methods of choice: Conjugate Gradients for positive definite problems and MINRES for indefinite problems. For these methods there exist descriptive convergence theories based on eigenvalues, i.e. convergence bounds given in terms of polynomial approximation problems on the eigenvalue spectrum which are often reasonably tight. A key consequence is that it is clear what one is trying to achieve to get fast convergence via preconditioning in these cases, namely well distributed eigenvalues or reduced spectral condition number.

By contrast, existing convergence bounds for Krylov subspace methods such as GMRES for real nonsymmetric linear systems give little mathematical guidance for the choice of preconditioner. In this talk we will introduce a desirable mathematical property of a preconditioner which guarantees that convergence of GMRES will essentially depend only on the eigenvalues of the preconditioned system, as is true in the symmetric case.

Minisymposium M9

High frequency and oscillatory problems

Organiser: Mark Ainsworth

Optimally blended finite element-spectral element schemes for wave propagation

Mark Ainsworth & Hafiz Wajid *(Strathclyde University)*

In an influential article, Marfurt suggested that the "best" scheme for computational wave propagation would involve an averaging of the consistent and lumped finite element approximations. Many authors have considered how this might be accomplished for first order approximation, but the case of higher orders remained unsolved. We describe work on the dispersive and dissipative properties of a novel scheme for computational wave propagation obtained by averaging the consistent (finite element) mass matrix and lumped (spectral element) mass matrix. The objective is to obtain a hybrid scheme whose dispersive accuracy is superior to both of the schemes. We present the optimal value of the averaging constant for all orders of finite elements and prove that for this value, the scheme is two orders more accurate compared with finite and spectral element schemes and, in addition, the absolute accuracy is of this scheme is better than that of finite and spectral element methods.

Recent Developments in nonpolynomial finite element methods for wave problems

T. Betcke & J. Phillips *(University College London)*

In recent years nonpolynomial finite element methods for the solution of frequency domain wave problems such as the Helmholtz equation have become of growing interest in Mathematics and Engineering. Based on oscillatory basis functions instead of polynomials they have the potential to lead to a significant decrease of the number of needed basis functions for a satisfactory accuracy for solutions of wave problems. In this talk we review some recent developments for nonpolynomial finite element methods and in particular focus on adaptivity and the behavior of these methods for inhomogeneous media problems.

Extremely Large Electromagnetics Problems: Are We Going in the Right Direction ?

Özgür Ergül & Levent Gürel *(University of Strathclyde)*

Recently, a popular approach for the solution of real-life electromagnetics problems is to use boundary-element methods with low-order discretizations. This strategy provides robust and flexible implementations allowing for the fast and accurate analysis of three-dimensional complicated objects with arbitrary geometries and electromagnetic excitations. Since accurate solutions via low-order elements require dense discretizations, matrix equations derived from real-life applications often involve millions of unknowns. In addition, as opposed to those derived from finite-element methods, these matrices are not sparse. Hence, recent studies in this area have mainly focussed on developing fast solvers, such as the multilevel fast multipole algorithm (MLFMA), and employing these low-complexity algorithms on parallel computers. In fact, the last decade has seen marvelous advances in this area leading to a rapid increase in the problem size from millions to more than one billion. The developed full-wave implementations have been used to solve extremely large electromagnetics problems involving complicated objects that are larger than 1000λ, where λ is the wavelength, on moderate computers with distributed-memory architectures.

Solutions of extremely large electromagnetics problems require a well designed combination of diverse components from different areas, such as numerical methods, fast algorithms, iterative solutions, parallelization, and high performance computing. Involving diverse components, the resulting simulation environments contain various error sources introduced at different stages. For example, parallel MLFMA implementations have the following error

sources, some of which are shared by other computational methods:

- Discretization of the three-dimensional model.
- Discretization of the integral-equation formulations.
- Numerical integrations on the discretization elements to calculate the near-zone interactions.
- Factorization of the far-zone interactions and truncation of the number of harmonics.
- Interpolations in multilevel interactions.

All these error sources make contributions to the final output, e.g., computed scattered or radiated electromagnetic fields. Recent works have focussed on increasing the problem size and the number of unknowns, but less attention has been paid to the accuracy of the results, particularly compared to alternative approximate techniques.

This study is on the accuracy of solutions of extremely large electromagnetics problems using a full wave solver based on MLFMA. We discuss the aforementioned error sources and their effects on the solutions. It is shown that the relaxation of some error sources would lead to more "efficient" solutions, as sometimes practiced in the literature. Unfortunately, such relaxation techniques may significantly deteriorate the accuracy of the results such that using a full-wave solver becomes meaningless. To encourage fair comparisons of the developed implementations for large-scale computations and emphasizing the accuracy of the results, we present a list of benchmark problems involving canonical objects of various sizes and their accurate solutions using a sophisticated implementation of MLFMA. Problems include a sphere with a diameter of 680λ and the NASA Almond that is larger than 1500λ. Both objects are discretized with more than 500 million unknowns and analyzed with maximum 1% error.

A high frequency boundary element method for scattering by non-convex obstacles

Steve Langdon, Simon Chandler-Wilde, Dave Hewett & Ashley Twigger *(University of Reading)*

Standard finite or boundary element approaches for the numerical solution of high frequency scattering problems, with piecewise polynomial approximation spaces, suffer from the limitation that the number of degrees of freedom required to maintain accuracy must increase at least linearly with respect to frequency in order to maintain accuracy. This can lead to excessively expensive computations at high frequencies. To reduce the computational cost, recent work has focused on the inclusion of oscillatory functions in the approximation space, so as to better represent the oscillatory solution. In this talk we review this approach as applied to some simple problems of scattering by convex obstacles, and we describe the extension of these ideas to more complicated problems of scattering by non-convex obstacles.

Minisymposium M10

Linear algebra in data-sparse representations

Organisers: Ivan Oseledets and Pavel Zhlobich

Tensor trains and high-dimensional problems

Ivan Oseledets *(Russian Academy of Sciences)*

In this talk, I will introduce *tensor train format*, or simply TT-format and explain, why it can be considered as one of the most promising low-parametric representations for high-dimensional problems in chemistry, physics and mathematics.

Rank-one QTT vectors with QTT rank-one and full-rank Fourier images

Dmitry Savostyanov *(Russian Academy of Sciences)*

Recently, fast algorithm was proposed for the Fourier transform and related sine/cosine transforms, using QTT format for data-sparse approximate representation of one– and multi–dimensional vectors (m-tensors). Although a Fourier matrix itself does not possess a low-rank QTT representation, it can be efficiently applied to m–tensor in the QTT format exploiting the multilevel structure of the Cooley-Tuckey algorithm. The m–dimensional Fourier transform of an $n\times\ldots\times n$ vector with $n = 2^d$ has $\log^2(\text{size}) = \mathcal{O}(m^2d^2r^3)$ complexity, where r is the maximum QTT rank of input, output and all intermediate vectors in the Cooley-Tuckey scheme. The storage size in QTT format is bounded by $\mathcal{O}(mdr^2)$.

The proposed FFT-QTT algorithm outperforms the FFT algorithm for vectors with large n and m and moderate r. It is instructive to describe such vectors more explicitely. In this talk we describe the class of QTT rank-one vectors with rank-one Fourier images. We also give an example of QTT rank-one vector that has the Fourier images with full QTT ranks.

In numerical experiments we show that the use of QTT format for such vectors relaxes the grid size constrains and allow high-resolution computations of Fourier images and convolutions in high dimensions without "curse of dimensionality".

Matrix computations with data in multi-index formats

E Tyrtyshnikov *(Russian Academy of Sciences)*

Vectors and matrices are usually considered as arrays with one or two indices. However, the same data can be easily viewed as arrays with more (artificial) indices, e.g. a vector of size $n = 2^d$ can be considered as an d-index array of size $2 \times \ldots \times 2$. When using recently proposed tensor-train decompositions one can design efficient algo-

rithms for basic matrix operations of complexity linear in d. Thus, the well-known *curse of dimensionality* converts into the *blessing of dimensionality*. The new approach puts forth many wonderful perspectives and questions for future research. Applications include spectral problems of computational chemistry, stochastic differential equations, general parametric problems, fast interpolation methods for multivariate data etc. The purpose of this talk is to outline the new tensor representation techniques, related theoretical findings and efficient algorithms reducing multidimensional computations to matrix ones, applications, on-going works and perspectives.

Minisymposium M11

Optimization: complexity and applications

Organiser: Peter Richtarik

The Fast Gradient Method as a Universal Optimal First-Order Method

Olivier Devolder, François Glineur and Yurii Nesterov *(Université Catholique de Louvain)*

The goal of this talk is to show that the fast-gradient method, initially designed for smooth convex optimization (convex functions with Lipschitz-continuous gradient), can be also applied to convex problems with weaker level of smoothness (including non-smooth problems with bounded subgradients) and provides for these classes an optimal first-order method.

A new definition of inexact oracle was previously introduced in order to study the behavior of the first-order methods of smooth convex optimization (classical and fast-gradient methods) when only approximate first-order information is available.

In this talk, we prove that an exact oracle of non-smooth convex optimization can be seen as an inexact oracle of smooth convex optimization. This observation gives us the possibility to apply the gradient and the fast-gradient methods to non-smooth functions, replacing gradients by subgradients and replacing the Lipschitz-constant of the gradient by a well-chosen quantity. We prove that these two adapted methods have a convergence rate of $O(\frac{1}{\sqrt{k}})$ on the non-smooth problems and are therefore optimal.

The same kind of results hold for weakly smooth functions (i.e. functions with Hölder-continuous gradient). We obtain that the fast-gradient method achieves the optimal rate of convergence for this class: $O\left(\frac{1}{k^{\frac{1+3\nu}{2}}}\right)$ where ν denotes the Hölder parameter.

Finally, we prove that the fast-gradient method can be applied to smooth and non-smooth strongly convex problems with here also an optimal complexity.

Solving topology optimization problems by domain decomposition

Michal Kocvara *(University of Birmingham)*

We investigate two approaches to the solution of topology optimization problems using decomposition of the computational domain. The first approach is based on a two stage algorithm. The basic method is the block Gauss-Seidel algorithm used in the same way as in domain decomposition methods for the solution of linear systems. Here, however, we apply the block Gauss-Seidel to a constraint optimization problem. It is well known that such a method, in general, does not converge to a critical point of the optimization problem. To guarantee convergence, we follow one iteration of the block Gauss-Seidel method by a few steps of a converging first-order method. We will show that the resulting two stage algorithm leads to a significant improvement in the solution efficiency. The second approach uses reformulation of the original problem as a semidefinite optimization problem. This approach is particularly suitable for problems with vibration or global buckling constraints. Standard semidefinite optimization solvers exercise high computational complexity when applied to problems with many variables and a large semidefinite constraint. To avoid this unfavorable situation, we use results from the graph theory that allow us to equivalently replace the original large-scale matrix constraint by several smaller constraints associated with the subdomains. This leads to a significant improvement in efficiency, as will be demonstrated by numerical examples. Joint work with M. Kojima (Tokyo Institute of Technology), D. Loghin and J. Turner (both University of Birmingham).

Efficiency of Randomized Coordinate Descent Methods on Minimization Problems with a Composite Objective Function

Martin Takáč & Peter Richtárik *(University of Edinburgh)*

We develop a randomized block-coordinate descent method for minimizing the sum of a smooth and a simple non-smooth block-separable convex function and prove that it obtains an ϵ-accurate solution with probability at least $1-\rho$ in at most $O((2n/\epsilon)\log(1/\epsilon\rho))$ iterations, where n is the dimension of the problem. This extends recent results of Nesterov (Efficiency of coordinate descent methods on huge-scale optimization problems, 2010), which cover the smooth case, to composite minimization, and improves the complexity by a factor of 4. In the smooth case we give a much simplified analysis. Finally, we demonstrate numerically that the algorithm is able to solve various ℓ_1-regularized optimization problems with a billion variables.

Minisymposium M12

Compressed Sensing: algorithms and theory

Organiser: Peter Richtarik

GPU Accelerated Greedy Algorithms for Sparse Approximation

Jeffrey Blanchard *(Grinnell College)*

Thresholding algorithms are efficient methods for determining the best k-term approximation of a given signal when an incomplete set of linear measurements is known. These greedy algorithms have been extensively tested on unrealistically small problems. We show the efficacy of GPU based greedy algorithms and observe speedups on a single Nvidia Tesla C2050 of 50 - 75 times a state of the art Intel Xeon 5650 CPU. These performance gains comes from both the GPU and alterations to the algorithms which exploit the properties of the GPU, and it enables testing of more realistic sized signals of length 10^6. This is joint work with Jared Tanner.

Compressed Sensing Thresholds and Condition Numbers in Optimization

Martin Lotz *(Univeristy of Edinburgh)*

We show how a precise error analysis of sparse recovery problems with noise can be obtained from the study of generalizations of Renegar's condition number for convex feasibility problems. The probability distribution of these condition measures for random problem instances is well studied, leading in turn to results on robust compressed sensing.

A GPU accelerated coordinate descent method for large-scale L1-regularized convex minimization

Peter Richtarik *(University of Edinburgh)*

Compared with an efficient CPU code, a GPU implementation of a coordinate descent method for L1-regularized convex optimization is capable of producing unprecedented speedup. Joint work with Martin Takac.

A new recovery analysis of Iterative Hard Thresholding for Compressed Sensing

Andrew Thompson *(University of Edinburgh)*

Compressed Sensing (CS) seeks to recover sparse or compressible signals from undersampled linear measurements - it asserts that the number of measurements should be proportional to the information content of the signal, rather than its dimension. One particular CS problem that has received much attention recently is that of recovering a k-sparse signal $x \in \mathbb{R}^N$ from n linear measurements, where $k \leq n \leq N$. Since the introduction of CS in 2004, many algorithms have been developed to solve this problem. Because of the paradoxical nature of CS - exact reconstruction from undersampled measurements - it is crucial for the acceptance of an algorithm that rigorous worst-case analysis verifies the degree of undersampling the algorithm permits. This aim can be accomplished by means of the phase transition framework in which we let $(k, n, N) \to \infty$, while preserving the proportions $\delta = n/N$ and $\rho = k/n$.

We provide a new worst-case analysis for one of these recovery algorithms, Iterative Hard Thresholding (IHT). For the specific case of Gaussian measurement matrices, comparison with existing results by means of the phase transition framework shows a substantial quantitative improvement. We derive two conditions for general measurement matrices: Firstly, by analysing the fixed points of IHT we obtain a condition guaranteeing at most one fixed point (namely the original signal). Secondly, we give an improved condition guaranteeing convergence to some fixed point. If both conditions are satisfied, it follows that we have guaranteed recovery of the original signal. A statistical analysis of the fixed point condition for Gaussian measurement matrices allows us to derive a quantitative phase transition.

We also extend the consideration to variants of IHT with variable step-size, including Normalized Iterative Hard Thresholding (NIHT). A similar analysis in this case yields a further significant improvement on the phase transition for Gaussian measurement matrices.

Abstracts of Contributed Talks

Reduction and solutions for unsteady flow of a Sisko fluid for cylindrical geometry

S Abelman *(University of the Witwatersrand)*

In this study some reductions and solutions for unsteady flow of a Sisko fluid are investigated. The governing nonlinear equation for unidirectional flow of a Sisko fluid is modelled in cylindrical polar coordinates. The exact steady-state solution for the nonlinear problem is obtained. The reduction of the governing nonlinear problem is carried out by using the similarity approach. Further, by time translation and scaling symmetries, the partial differential equation is transformed into an ordinary differential equation, which is integrated numerically taking into account the influence of the index n and the material parameter b of the Sisko fluid. A comparison between profiles of Newtonian and Sisko fluids is presented.

Bernstein-Bézier Finite Elements

Gaelle Andriamaro, Mark Ainsworth & Oleg Davydov *(University of Strathclyde)*

Algorithms with optimal complexity are presented for the computation of the element mass and stiffness matrices for finite element spaces based on Bernstein-Bézier polynomials which, for a given simplex $T \subseteq \mathbb{R}^d$, are defined by

$$B^n_{\boldsymbol{\alpha}} = \binom{n}{\boldsymbol{\alpha}} \boldsymbol{\lambda}^{\boldsymbol{\alpha}}, \quad \boldsymbol{\alpha} \in \mathcal{I}^n_d,$$

where $\mathcal{I}^n_d$ is the set of non-negative integer $(d+1)$-tuples which sum up to n, and $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_{d+1})$ is the set of barycentric coordinates with respect to T. Although the Bernstein polynomials have several properties which make them intensively used in computationally demanding applications such as CAGD and visualisation, they have received little attention from the finite element community. The degrees of freedom corresponding to the obtained basis are completely symmetrical, and the presented elements are the first to achieve optimal complexity on simplicial elements.

The complexity needed to assemble the element matrices for the Bernstein polynomials is optimized using a remarkable feature of the Bernstein polynomials: Although not based on a tensorial construction, the Bernstein-Bézier basis possesses the key properties needed for the sum factorization techniques. In addition, the product of two Bernstein polynomials is again a Bernstein polynomial, which reduces the entries of the element matrices to components of the moment vector $\mu^\nu_{\boldsymbol{\alpha}}(\mathbf{f}) = \int_T f(\mathbf{x}) B^\nu_{\boldsymbol{\alpha}}(\mathbf{x}) \mathrm{d}\mathbf{x}$, $\boldsymbol{\alpha} \in \mathcal{I}^\nu_d$, for appropriate ν, for example $\nu = 2n-2$ for the the components of the stiffness matrix.

Discontinuous Galerkin methods for time-dependent advection dominated optimal control problems

Tuğba Akman, Hamdullah Yücel & Bülent Karasözen *(Middle East Technical University)*

We consider optimal control problems (OCPs) governed by time-dependent diffusion-advection-reaction equations with distributed controls. For the numerical solution of the OCP, we use the *discretize-then-optimize* approach. It is well known that the standard finite element discretizations applied to convection dominated diffusion problems lead to strongly oscillations; the interior and boundary layers can not be resolved properly. Several well-established stabilization techniques have been proposed and applied in the literature. In contrast to the these, the discontinuous Galerkin finite element method (DGFEM) provides accurate solutions for convection dominated problems. Recently several methods were applied for stationary convection dominated OCPs, but there exists few works for time-dependent problems. The state, adjoint and control variables are discretized in space by the symmetric (SIPG), the nonsymmetric (NIPG) and the incomplete (IIPG) interior penalty Galerkin methods. For the temporal discretization, backward Euler, Crank-Nicolson and semi-implicit method are used. The resulting OCP has been solved by the Newton-conjugate gradient, limited BFGS and the steepest descent method. The numerically obtained converge orders for the cost function confirm the a priori error estimates.

DRBEM and DQM Solutions of Natural Convection Flow in a Cavity Under a Magnetic Field

Nagehan Akgün & Münevver Tezer Sezgin *(Middle East Technical University)*

In this paper, the dual reciprocity boundary element method (DRBEM) and the differential quadrature method (DQM) are applied to solve the two-dimensional, unsteady natural convection flow in a square cavity under an externally applied magnetic field. The governing equations are given in terms of stream function (ψ), vorticity (w) and temperature (T) as

$$\begin{aligned} \nabla^2 \psi &= -w \\ Pr \nabla^2 w &= \frac{\partial w}{\partial t} + u\frac{\partial w}{\partial x} + v\frac{\partial w}{\partial y} + Ha^2 Pr \frac{\partial v}{\partial x} - RaPr\frac{\partial T}{\partial x} \\ \nabla^2 T &= \frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} \end{aligned} \tag{6}$$

where $u = \dfrac{\partial \psi}{\partial y}$, $v = -\dfrac{\partial \psi}{\partial x}$ are velocity components, Pr, Ha and Ra are the Prandtl number, Hartmann number and Rayleigh number, respectively. Vorticity transport and energy equations are transformed to the form of modified Helmholtz equations by utilizing forward difference with relaxation parameters for the time derivatives, and approximating also Laplacian terms at two consecutive

time levels. In the DRBEM solution the resulting modified Helmholtz equations are solved by using the fundamental solution $\frac{1}{2\pi}K_0(x)$ of the modified Helmholtz equation whereas in the stream function Poisson's equation $\frac{1}{2\pi}\ln(x)$ (the fundamental solution of Laplace equation) is made use of. In the DQM solution also these modified Helmholtz equation are used keeping all the previous time level terms as inhomogeneity. In both DRBEM and DQM procedures since the equations are solved in terms of modified Helmholtz equations containing the time advancement in it, there is no need to use another time integration scheme, and one has the advantage of using large time increments. In the DQM solution procedure Gauss-Chebyshev-Lobatto space points are used which are clustered through the end points. The comparison between the DRBEM and DQM solutions are made in terms of computational cost and accuracy. DQM has the advantage of using very small number of discretization points, and giving accurate and efficient solutions. Both DQM and DRBEM are applied on the natural convection flow under a magnetic field in a square cavity heated and cooled on the vertical walls, and adiabatic conditions imposed on the horizontal walls. Solutions are obtained for Rayleigh number values between 10^3 and 10^6, and Hartmann numbers up to $Ha = 300$. Although, DRBEM and DQM give almost the same accuracy, DQM is desirable since it uses considerably small number of grid points resulting with less computational work.

Convergence Analysis of a Family of Damped Quasi-Newton Methods for Nonlinear Optimization

Mehiddin Al-Baali *(Sultan Qaboos University)*

In this talk we will extend the technique in the damped BFGS method of Powell (Algorithms for nonlinear constraints that use Lagrange functions, Mathematical Programming, 14: 224–248, 1978) to a family of quasi-Newton methods with applications to unconstrained optimization problems. An appropriate way for defining this damped-technique will be considered to enforce safely the positive definiteness property for both positive and indefinite quasi-Newton updates. It will be shown that this technique maintains the global and superlinear convergence property of a restricted class of quasi-Newton methods for convex functions. This property will be also enforced for an interval of divergent quasi-Newton methods. Numerical experiences will be described to show that the proposed technique improves the performance of quasi-Newton methods substantially and significantly in certain robust and inefficient cases (eg, the BFGS and DFP methods), respectively.

How to solve boundary value problems by using Variational Iteration Method

Derya Altıntan & Ömür Uğur *(Middle East Technical University)*

Many problems of science are represented by a system of linear or nonlinear differential equations. It is in general difficult to solve such type of systems and, hence, finding approximate or, if possible, closed-form solutions has been the subject of many researchers. The Variational Iteration Method (VIM) is an alternative to numerically solving those equations and has proven its applicability. The method constructs a correction functional by using Lagrange multipliers which will be identified by using calculus of variations and restricted variations. We study the method for solving boundary value problems, and obtain a relation between the Lagrange multipliers and the corresponding adjoint differential equation. Furthermore, we obtain the generalisation of the method to the matrix-valued Lagrange multipliers, and hence, enjoy the usage of no restricted variations in the linear part of the splitting operator. To illustrate the method we apply method to various systems.

Stability and convergence of finite difference schemes for complex diffusion processes

Adérito Araújo, Sílvia Barbeiro & Pedro Serranho *(University of Coimbra)*

Diffusion processes are commonly used in image processing in order to remove noise. The main idea is that if one pixel is affected by noise, than the noise should be diffused among the neighboring pixels in order to smooth the region. In this way proper diffusion partial differential equations have been considered to achieve this end. Taking the heat equation

$$\frac{\partial u(x,t)}{\partial t} = \nabla \cdot (D(x,t,u)\nabla u(x,t))$$

where $u(x,t)$ represents the denoised image at time t with the initial noisy image $u(x,0)$, the choice of the diffusion parameter D plays a very important role for the purpose of denoising. Roughly speaking, one wants D to allow diffusion on homogeneous areas affected only by noise and to forbid diffusion on edges to preserve features of the original denoised image. In this way, several expressions for D have been suggested.

The first approaches indicated that D should depend on the gradient of u with an inverse proportion. However, this approach had a few handicaps. For instance, within a ramp edge the diffusion coefficient is similar along all the edge delaying the diffusion process, not distinguishing between the end points and interior points of the ramp edge where diffusion should differ. Therefore, the use of the laplacian was suggested as being more appropriate since it has a higher amplitude near the end points and low magnitude elsewhere. The drawback is that the computation of a higher order derivative is needed leading to higher ill-posedness in the first steps while the image is strongly affected by noise. To overcome this problem, some authors suggested to use complex diffusion. The use of a complex diffusion coefficient turns the partial differential equation into some sort of combination between the heat and the Schrödinger equation.

In recent years, nonlinear complex diffusion proved to be a numerically well conditioned technique that have been successfully applied in medical imaging despeckling and denoising. The main purpose of this work is to obtain a stability condition and establish to prove the conver-

gence for a class on finite difference schemes for a nonlinear complex diffusion equation. Some numerical results, obtained in the context of a collaboration with the Institute of Biomedical Research in Light and Image (IBILI), a research institution of the Faculty of Medicine of the University of Coimbra, are also presented.

A posteriori error estimation for coupled problems

Liya Asner, Simon Tavener & David Kay *(University of Oxford)*

The coupling of multi-physics systems is essential for a variety of problems arising in engineering and applied science. Given their scale and complexity, such problems are usually solved numerically, often using finite element methods. It is important to verify the accuracy of the obtained approximate solutions, for instance if the computational model in question aids decision-making in a clinical setting. *A posteriori* methods provide an efficient practical tool for error estimation. They can also be used to drive mesh refinement algorithms, which minimize the error given limited computational resources.
We present an *a posteriori* error representation formula for a time-dependent coupled problem. The representation relies on the solution of a dual problem. Both systems are solved using a finite element method with Lagrange multipliers, so that the system remains fully coupled and the method stability is not compromised. The accuracy of the representation formula is verified for regular quantities of interest. A space-time mesh refinement strategy based on local error estimates is proposed. The effectivity of the representation formula and the performance of the mesh refinement algorithm are tested numerically in a number of two-dimensional test problems. In particular, we consider a travelling solution, and show that its non-trivial behaviour is captured. The meshes produced using the developed strategy require a significantly lower number of degrees of freedom than the uniform meshes, which achieve similar accuracy.

A low order local projection stabilized finite element method for the Oseen equation

Gabriel R. Barrenechea & Frédéric Valentin *(University of Strathclyde)*

This talk is devoted to describe a new local projection stabilized finite element method (LPS) for the Oseen problem. The method adds to the Galerkin formulation new fluctuation terms which are symmetric and easily computable at the element level. Proposed for the pair $\mathbb{P}_1/\mathbb{P}_l$, $l = 0$, 1, when the pressure is continuously or discontinuously approximated, well-posedeness and error optimality are proved. In addition, we introduce a cheap strategy to recover an element-wise mass conservative velocity field in the discontinuous pressure case, a property usually neglected in the stabilized finite element context. Numerics validate the theoretical results and show that the present method improves accuracy to represent boundary layers when compared with alternative approaches.

A formula for the influence of jumps on finite sinc interpolants

Jean–Paul Berrut *(Université de Fribourg)*

In an article that appeared in "Numerical Algorithms" in 2007, we have discovered that a sinc interpolant on a finite interval essentially is the product of a harmonic function by the difference of two quadrature formulae for a Cauchy principal value integral. In a second paper in the same journal, that appeared recently, we have proved an Euler–Maclaurin formula for the error of such quadratures in the presence of jumps of the integrand.

The present work combines the two results to obtain a formula that quantifies the impact of an arbitrary number jumps on finite sinc interpolants. Numerical results show that the application of the formula, together with a quotienting method against the Gibbs phenomenon, allows for a spectacular damping, when not total elimination, of this impact.

Differential complexes and interpolation operators in the context of high-order numerical methods for electromagnetic problems

Alex Bespalov & N Heuer *(University of Manchester)*

It is now well known that differential complexes (or, exact sequences of vector spaces and differential operators), e.g.,

$$H^1 \xrightarrow{\nabla} \mathbf{H}(\mathrm{curl}) \xrightarrow{\mathrm{curl}} L^2,$$

are important in the analysis of time-harmonic problems of electromagnetics.

When discretising these problems, it is equally important to use the approximation spaces forming the corresponding discrete sub-complexes. This leads to stable discretisations enjoying some local conservation properties. For instance, a discrete counterpart of the above exact sequence is

$$X_N^1 \xrightarrow{\nabla} \mathbf{X}_N^{\mathrm{Ned}} \xrightarrow{\mathrm{curl}} X_N^0,$$

where X_N^1 is the space of continuous piecewise polynomials, $\mathbf{X}_N^{\mathrm{Ned}}$ is the $\mathbf{H}(\mathrm{curl})$-conforming finite element space based on the first Nédélec family, and X_N^0 is the space of piecewise (possibly discontinuous) polynomials (here, N is a generic discretisation parameter).

The continuous and discrete complexes linked by interpolation operators (projectors) form de Rham diagram, which commutes if the discrete spaces and interpolation operators are chosen properly. The commuting diagram property, and the corresponding error estimates for interpolation operators, have immediate applications to the numerical analysis of time-harmonic electromagnetic problems. In particular, these results are critical to prove the discrete compactness property, which in turn implies the convergence of approximations, as well as for the error analysis.

In this talk, we demonstrate how the above constructions are applicable to numerical analysis of the electric field integral equation in three dimensions. We focus on the boundary element discretisations employing high-order

polynomials (i.e., p- and hp-versions of the boundary element method). Inspired by the work of Demkowicz and Babuška on high-order finite element approximations of Maxwell's equations, we introduce and analyse a new projection based interpolation operator which satisfies the commuting diagram property involving appropriate trace spaces. We also establish an estimate for the interpolation error in the norm of the trace space $\tilde{\mathbf{H}}^{-1/2}(\div)$, which is closely related to the energy spaces for boundary integral formulations of time-harmonic problems of electromagnetics in three dimensions.

Nonlinear functional equations satisfied by orthogonal polynomials

C. Brezinski, *(Université des Sciences et Technologies de Lille)*

Let c be a linear functional defined by its moments $c(x^i) = c_i$ for $i = 0, 1, \ldots$. We proved that the nonlinear functional equations $P(t) = c(P(x)P(\alpha x + t))$ and $P(t) = c(P(x)P(xt))$ admit polynomial solutions which are the polynomials belonging to the family of formal orthogonal polynomials with respect to a linear functional related to c. This equation relates the polynomials of the family with those of the scaled and shifted family. Other types of nonlinear functional equations whose solutions are formal orthogonal polynomials are also presented. Applications to Legendre and Chebyshev polynomials are given. Then, orthogonality with respect to a definite inner product is studied. When c is an integral functional with respect to a weight function, the preceding functional equations are nonlinear integral equations, and these results lead to new characterizations of orthogonal polynomials on the real line, on the unit circle, and, more generally, on an algebraic curve.

On numerical algorithms for level set and curvature based models for surface fairing

Carlos Brito-Loeza *(Universidad Autónoma de Yucatán and University of Liverpool)*

The problem of surface fairing has been successfully addressed using variational models. To this end, different models involving the minimization of different functionals, some using the Gaussian curvature of the surface, others the mean curvature and the rest using variations or combinations of the principal curvatures of the surface has been proposed and tested by different authors. Either way using an implicit representation of the surface by level sets or an explicit representation by triangulation, a usually stiff and high order partial differential equation arising from the minimization problem has to be solved. So far the explicit representation is more popular particularly within the computer graphics community since apparently it delivers a faster numerical solution than the level set method. For the latter and up to our knowledge only a explicit Euler method has been reported in the literature. In this talk we will present our success in using the stabilized fixed point method proposed in [C. Brito-Loeza and K. Chen, *Multigrid algorithm for high order denoising*, SIAM J. Imaging Sci., 3 (2010), pp. 363-389.] to rapidly find the solution of the model $\int_\Omega h^2 |\nabla\Phi| d\Omega$ where $h = \nabla \cdot \frac{\nabla\Phi}{|\nabla\Phi|}$ stands for the mean curvature of the surface represented by the zero level set of Φ. We will also discuss our experiences in applying the same algorithm to the model presented in [Matthew Elsey and Selim Esedoglu, *Analogue of the total variation denoising model in the context of geometry processing*, SIAM Multiscale Model. Simul., 7 (2009), pp. 1549-1573]

Using reduced-order models and waveform relaxation to solve cerebral bloodflow autoregulation DEs on a large binary tree network

Richard Brown & Tim David *(University of Canterbury)*

Under certain assumptions the network of cerebral blood vessels can be modelled by a purely resistive binary tree where each vessel is characterised by a single resistance, computed as a function of its length and radius. Each vessel has the ability to vasoconstrict or vasodilate, hence changing their resistance, in response to local variables such as cellular Ca2+ concentration within the vessel, and collectively they autoregulate the cerebral bloodflow. These dynamics are highly nonlinear and can be described phenomenologically by a system of ODEs for each vessel.

Mathematically, the overall system is a large network of coupled ODEs, which can comprise up to millions of variables. The overall system is highly coupled, and can exhibit stiffness, so solving by traditional sequential ODE algorithms can be very expensive. The tree structure suggests an obvious parallelisation of the problem into subtrees, where the coupling between subtrees can be captured by a single variable: the blood pressure $p_i(t)$ at the junction where the trees are coupled. The system can be solved iteratively by a waveform relaxation variant, however convergence can be very slow. To speed up convergence we investigate using a small linear reduced order model obtained from a linearisation of the overall system to get a close initial approximation to start the waveform relaxation procedure.

Mimetic Finite Difference methods for elliptic problems

Andrea Cangiani *(University of Leicester)*

In this talk we present recent developments in Mimetic Finite Difference (MFD) methods for elliptic problems. MFD methods, at least in their low order, original, versions are techniques to extend classical finite element methods to general polygonal/polyhedral meshes. General meshes arise in the treatment of complex solution domains and heterogeneous materials (e.g. reservoir models) and are particularly indicated in moving meshes techniques as well as adaptive mesh refinement/de-refinement.

A more well known technique to extend finite elements to polygonal meshes is given by harmonic finite elements. We will present a novel interpretation of MFDs showing that these combine the accuracy and ease of implemen-

tation of standard, polynomial finite elements, with the meshing flexibility of harmonic elements. We shall also describe MFDs for elliptic eigenvalue problems as well as convection-diffusion problems. Stabilization techniques in the convection-dominated regimes will also be presented.

Convolution quadrature revisited for Volterra integral equations

Penny J Davies & Dugald B Duncan *(University of Strathclyde)*

Convolution quadrature (CQ) methods were introduced by Lubich in 1988 to approximate convolution integrals. More recently they have been used for the temporal approximation of time–dependent boundary integral equations together with a finite element or collocation approximation in space, because they typically give a more stable numerical algorithm than standard time-stepping methods. The drawback is that the support of the associated CQ basis functions is infinite, which gives rise to dense system matrices and makes the method inefficient. We show how using a spline-based implementation of the CQ methodology can circumvent this.

RBF-FD Methods for Elliptic Equations

Oleg Davydov & Dang Thi Oanh *(University of Strathclyde)*

We investigate low order RBF-based generalised finite difference methods (RBF-FD) on irregular centres. This approach is genuinely meshless and can compete in accuracy with the linear finite element method that requires solving linear systems of comparable bandwidth/density. Algorithms and numerical results for stencil support selection, adaptive refinement and optimal shape parameter will be discussed.

Postprocessing Reservoir Simulations to Obtain Accurate Well Pressures

Dugald B Duncan & Nneoma Ogbonna *(Heriot-Watt University)*

We discuss a new post-processing technique for standard reservoir simulators to efficiently determine detailed and accurate information about the time-dependent pressure at a wellbore. This information is important in monitoring and assessing the properties and capacity of reservoirs of various types. The wellbore is a relatively tiny hole in a large reservoir. Standard simulators use point or line source well models and do not resolve down to the tiny scale of the well radius, which is where the required information actually is. Our method involves just a local solve of the time dependent pressure equation in the vicinity of the wellbore, using as boundary data information from the main reservoir simulation. We describe the connection with the widely used Peaceman wellbore index and its variants, discuss the accuracy (both from analysis and experiments) and show results from a number of test cases.

Comparing two iterated projection approximations for integral operators in terms of convergence and computational cost

Rosário Fernandes, Mario Ahues & Filomena d'Almeida *(Universidade do Minho)*

We will consider the Fredholm integral equation of the second kind

$$(T - zI)\varphi = f, \tag{7}$$

where T is a compact linear operator defined in a Hilbert space X by

$$(T\varphi)(s) = \int_a^b k(s,t)\varphi(t)dt,\ s \in [a,b],\ \varphi \in X,$$

I denotes the identity operator on X, z belongs to the resolvent set of T and f belongs to X.

An approximate solution of the equation (1) can be obtained as a solution of an approximate problem

$$(T_n - zI)\varphi_n = f, \tag{8}$$

where T_n is one element of a sequence $(T_n)_{n\geq 1}$ which is $\nu-$convergent to T.

This sequence can be obtained by projection methods, such as the Classical Galerkin, the Kantorovich or the Sloan methods. Given π_n a projection from X onto a finite dimentional subspace X_n, those approximations may be defined as $T_n^G = \pi_n T \pi_n$, $T_n^K = \pi_n T$ and $T_n^S = T\pi_n$, respectively.

Recently, R. Kulkarni has proposed a new projection method defined by $T_n^R = T_n^K + T_n^S - T_n^G$ and proved that, although the size of the linear system to be solved is the same as in the Galerkin method, the rate of convergence of the method proposed is higher than the order of the Classical Galerkin and the Sloan methods.

We will compare this method with the iterated Kantorovich approximation, both from the convergence point of view and their computational cost. When we mention iterated Kantorovich method we mean that we solve the approximate problem (11) thus obtaining φ_n^K and then we refine it using (10) that yields $\varphi_n^{IK} = \frac{1}{z}(T\varphi_n^K - f)$.

From all standard projection approximations of a bounded linear operator in a Hilbert space, iterated projection and Kulkarni's discretization exhibit a global superconvergent error bound.

Limited memory spectral gradient methods

Roger Fletcher *(University of Dundee)*

Spectral Gradient methods such as the Barzilai-Borwein method have given new impetus to the capability of solving large scale unconstrained optimization methods. The talk will described how significant improvements can be obtained by making use of a few extra 'long vectors' of memory. The possible application of these ideas to nonlinearly constrained optimization will also be explored.

Energy Conservation Laws of Maxwell's Equations and Their Application in Numerical Analysis of FDTD

Liping Gao *(China University of Petroleum)*

In this talk, I would like to introduce some new energy conservation laws of the 3D Maxwell's equations in time domain in the case of the perfectly electric conducting boundary conditions. Based on these new continuous forms of identities for the Maxwell's equations, discrete forms of identities for FDTD are derived, which show that FDTD is energy conserved in terms of the discrete H^1 norms. Conditional stability of FDTD in the discrete H^1 norms is then proved. By the energy-conserved identities of FDTD, we also prove that FDTD are second order accurate both in time and space in the discrete H^1 norms when a condition that is stronger than the CFL condition is satisfied. This means that FDTD is super convergent in the discrete H^1 norms. Numerical experiments are carried out and computational results to test the energy conservation, stability and super convergence are presented.

Puiseux-based extrapolation for large-scale degenerate quadratic programming

Nick Gould, Dominique Orban & Daniel Robinson *(STFC-Rutherford Appleton Laboratory)*

We describe the design of a new software package CQP for large-scale convex quadratic programming. The method is based on high-order Taylor and Puiseux approximation to a variety of infeasible arcs connecting the current iterate to a better target point. Possible arcs include those by Zhang and by Zhou and Sun based on work by Stoer, Mizuno, Potra and others. The resulting algorithm is provably both globally and polynomially convergent at an ultimately high-order (depending on the series used) in both non-degenerate and degenerate cases. We will illustrate a number of algorithmic options on the CUTEr QP test set. CQP is available as part of the fortran 90 library GALAHAD.

A parallel integrator for linear initial-value problems

Stefan Güttel & Martin J. Gander *(University of Oxford)*

We propose a novel parallel method for the integration of linear initial-value problems

$$u'(t) = Au(t) + f(t), \quad u(0) = u_0, \tag{9}$$

where A is a large sparse or structured matrix, and u, f are vectors depending on time. As opposed to most existing parallel methods which exploit the linear structure of (9), our method does not require direct or inverse Laplace transforms of f. We utilize an overlapping time decomposition of (9) into decoupled inhomogeneous and homogeneous subproblems, and a near-optimal Krylov method for the fast exponential propagation of the homogeneous subproblems. The solution of the original problem is then obtained by the superposition of subproblem solutions. The parallel speedup depends on the ratio by which homogeneous problems can be solved faster than inhomogeneous problems, and hence becomes large when the inhomogeneity f is sufficiently stiff. The efficiency of this approach is demonstrated at some model problems.

Matrix-free IPM with GPU acceleration

J.A.J. Hall, J. Gondzio & E. Smith *(University of Edinburgh)*

Interior point methods (IPM) with direct solution of the underlying linear systems of equations have been used successfully to solve very large scale linear programming (LP) and quadratic programming (QP) problems. However, the limitations of direct methods for some classes of problems have led to iterative techniques being considered. The *matrix-free* method is one such approach and is so named since the iterative solution procedure requires only the results of operations $A\mathbf{x}$ and $A^T\mathbf{y}$, where A is the matrix of constraint coefficients. Thus, in principle, it may be applied to problems where A is not known and only an oracle is available for computing $A\mathbf{x}$ and $A^T\mathbf{y}$. Since the computational cost of these operations may well dominate the total solution time for the problem, it is important that the techniques used to perform them are efficient.

This talk will outline the matrix-free interior point method and, for several classes of LP problems, demonstrate its overwhelmingly superior performance relative to the simplex method and IPM with equations solved directly. The dominant cost of the operations $A\mathbf{x}$ and $A^T\mathbf{y}$ will then be used to motivate their implementation on a GPU to yield further performance gains. Different computational schemes for these sparse matrix-vector products will be discussed. A comparison of the speed-up achieved using a many-core GPU implementation with that for a multi-core CPU implementation indicates the former has better potential.

Experience of linear solvers in an nonlinear interior point method

Jonathan Hogg *(STFC Rutherford Appleton Laboratory)*

We present the results of some extensive testing of various symmetric indefinite factorization codes inside the well-known nonlinear interior point solver IPOPT. We describe various experiments to improve performance and attempts to classify the problems on which each solver performs best.

In addition to the solvers that are available as standard we also give results on the latest HSL solvers aimed at multicore platforms.

A fast matrix assembling for interior penalty discontinuous Galerkin method

Tamás L. Horváth *(Széchenyi University)*

We investigate the matrix assembling for the IPDG solution of

$$-\nabla \cdot (A\nabla u) + B \cdot \nabla u = f \text{ on } \Omega,$$

$$u|_{\partial\Omega} = u_D,$$

with A and B piecewise constant. Using IPDG method we have to solve the following: find $w \in V_{DG}$ with $a(w,v)+b(w,v) = \varphi(v)$, $\forall v \in V_{DG}$ where:

$$\begin{aligned} a(w,v) &= \sum_{E\in\tau_h}\int_E A\nabla w\cdot\nabla v - \sum_{e\in\Gamma_0}\int_e \{\!\{A\nabla w\cdot\eta_e\}\!\}\,[\![v]\!] + \\ &\quad \epsilon\sum_{e\in\Gamma_0}\int_e \{\!\{A\nabla v\cdot\eta_e\}\!\}\,[\![w]\!] + \sum_{e\in\Gamma_0}\frac{\sigma_0}{|e|}\int_e [\![v]\!]\,[\![w]\!], \end{aligned}$$

$$b(w,v) = -\sum_{E\in\tau_h}\int_E wB\cdot\nabla v + \sum_{e\in\Gamma_0}\int_e B\cdot\eta_e w^{up}\,[\![v]\!],$$

$$\varphi(v) = \int_\Omega fv + \sum_{e\in\Gamma}\int_e \left(\epsilon A\nabla v\cdot\eta_e + \frac{\sigma_0}{|e|}v + B\cdot\eta_e v\right) u_D,$$

where $[\![u]\!]$ is the jump of u, $\{\!\{u\}\!\}$ is the average of u on the interelement faces. τ_h denotes a triangular tessellation of Ω, $\Gamma = \partial\Omega$, $\Gamma_0 = \bigcup_{E\in\tau_h}\partial E$, σ_0 is the penalty parameter, $\varepsilon \in \{-1,0,1\}$ and V_{DG} contains polynomials of a given order on each element.

To set up the linear equations we have to compute $a(\Phi_i,\Phi_j)$ for the basis functions of V_{DG}. The computation of the corresponding integrals element-by-element is quite expensive especially if we are using higher order elements.

Standard reference domain based computations are well known for matrix assembling in comforming finite element procedures for constant diffusion matrices. These require only an affine linear mapping between the reference domain and the actual one and the integrals of the basis functions on the reference domain. For interior penalty the main difficulties emerge when calculating the integrals of jumps and averages on interelement faces.

These terms can be rewritten in a more convenient form without jumps and averages, see e.g. the book by Riviére. To calculate these integrals one should invest huge computational work for computing the quadrature points and evaluate the basis functions here.

To overcome these difficulties we develop a reference domain based algorithm, where we could calculate integrals on a reference domain and on its neighbours, and we only have to use the matrices containing these information. The advantage of our approach becomes clear when we are using higher order elements. The running times we present prove the efficiency of the method both in two and three dimensions.

A high performance dual simplex solver

Q. Huangfu & J.A.J. Hall *(University of Edinburgh)*

The dual simplex method is frequently the preferred approach when solving large scale linear programming (LP) problems. Algorithmic enhancements of the dual simplex method that are important for its efficient serial implementation are the dual steepest-edge framework and bound flipping ratio test. As the improved performance of modern computer architectures is now being achieved via parallelism, it is important that this be exploited by the dual simplex method. Suboptimization is a relatively unknown algorithmic variant of the dual simplex method that significantly increases the scope for exploiting parallelism. This talk will discuss how these three algorithmic enhancements may be combined within a parallel implementation by means of novel computational techniques. Results will be given that demonstrate the competitiveness of this implementation relative to an efficient serial dual simplex solver.

Zeros of matrix polynomials: A case study

Drahoslava Janovská & Gerhard Opfer *(Institute of Chemical Technology, Prague)*

Let us consider a matrix polynomial $\mathbf{p}$,

$$\mathbf{p}(\mathbf{X}) = \sum_{j=0}^{N}\mathbf{A}_j\mathbf{X}^j\mathbf{B}_j, \qquad \text{where}$$

$$\mathbf{X},\ \mathbf{A}_j,\ \mathbf{B}_j \in \mathbb{K}^{2\times 2}, \quad j=0,\dots,N, \quad \mathbf{A}_0\mathbf{B}_0,\ \mathbf{A}_N,\ \mathbf{B}_N \neq \mathbf{0},$$

$\mathbb{K}$ stands for the field of real or complex numbers, the matrices $\mathbf{A}_j$, $\mathbf{B}_j$, $j=0,1,\dots,N$, $N \geq 1$, are given matrices of order 2. If the matrix $\mathbf{X}$ has property that $\mathbf{p}(\mathbf{X}) = \mathbf{0}$, we call $\mathbf{X}$ a zero of $\mathbf{p}$. In general, the polynomial can consist of multiple terms of the same degree.

Let $\mathbf{X} \in \mathbb{K}^{2\times 2}$ and let $\chi_{\mathbf{X}}(z) = z^2 - \mathrm{tr}(\mathbf{X})\,z + \det(\mathbf{X})$ be its characteristic polynomial. Then there exist numbers $\alpha_j,\ \beta_j,\ j=0,1,\dots,$ such that $j-$power of the matrix $\mathbf{X}$ can be written as

$$\mathbf{X}^j = \alpha_j\mathbf{X} + \beta_j\mathbf{I} \quad \text{for all } j=0,1,\dots, \text{ where } \alpha_0 := 0,\ \beta_0 := 1,$$

$$\alpha_{j+1} := \mathrm{tr}(\mathbf{X})\alpha_j + \beta_j, \quad \beta_{j+1} := -\alpha_j\det(\mathbf{X}), \quad j \geq 0,$$

and the polynom $\mathbf{p}$ has the form

$$\begin{aligned} \mathbf{p}(\mathbf{X}) &= \sum_{j=0}^{N}\mathbf{A}_j(\alpha_j\mathbf{X} + \beta_j\mathbf{I})\mathbf{B}_j \\ &= \mathbf{A}_0\mathbf{B}_0 + \sum_{j=1}^{N}\alpha_j\mathbf{A}_j\mathbf{X}\mathbf{B}_j + \sum_{j=2}^{N}\beta_j\mathbf{A}_j\mathbf{B}_j. \end{aligned}$$

In this particular case, i.e. for $\mathbf{X},\ \mathbf{A}_j,\ \mathbf{B}_j \in \mathbb{K}^{2\times 2}$, we give a classification of all zeros of the polynomial in terms of the rank of the corresponding system. We have also developed an algorithm for the computation of these zeros.

In two papers [1], [2], quaternionic polynomials, both simple and two-sided, are investigated. Due to the fact that there is a class of 2×2 complex matrices and a class of 4×4 real matrices, which isomorphically represent quaternions, the quaternionic polynomials are implicitly contained in the investigation of matrix polynomials. In [1] we have shown that for one-sided quaternionic polynomials there are two classes of zeros: isolated and spherical. Two-sideded quaternionic polynomials have, in addition,

three more classes of zeros defined by the rank of a certain real 4×4 matrix, [2].

These two special examples of matrix polynomials show that the task to classify and compute zeros of the matrix polynomials is quite complicated even when the coefficients and unknown matrices are only of order two.

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On periodic patterns in the traffic flow

Vladimír Janovský & Lubor Buřič *(Charles University)*

We investigate microscopic models of the road traffic, see e.g. [1]. In particular, we consider a *car-following* model for a single-line traffic flow on a circular road, [2]. The model is characterized by a choice of a particular *optimal velocity function* (OV) which is related to each individual driver. The aim is to investigate *traffic jams*. Mathematically, the jams are periodic solutions of the model. They form smooth rotating waves. In [3], it was shown that periodic solutions (cycles) of the model are due to the Hopf bifurcation of steady state solutions. Nevertheless, one can check that many cycles become *non physical* for large parameter regions.

The analysis shows that a trajectory becomes non physical since an event which can be interpreted as a collision with the foregoing car. The natural action of a driver at that moment would be to overtake the slower car. In [4], we proposed a model of an overtaking. It *implicitly* defines a maneuver consisting of deceleration/acceleration just shortly before/after the event. The maneuver is fully defined by the OV of the driver. The resulting model is an *event-driven* model. It is no longer smooth. In [4], we also hinted at a large variety of oscillatory solutions (*oscillatory patterns*) of this new model.

In our presentation, we

- formulate our model as a particular *Filippov system*, see [5],
- define selected oscillatory patterns as invariant objects of this Filippov system,
- use the standard software (AUTO97) to continue these patterns with respect to a parameter,
- consider bifurcations of the patterns.

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The Effects of Dispersive and Dissipative Properties of Numerical Methods on the Linear Advection Equation during Data Assimilation

Siân Jenkins, Chris Budd, Melina Freitag & Nathan Smith *(University of Bath)*

Data assimilation is a method often used in forecasting where the results from a numerical model simulating a physical system are compared to past observations of the true physical system. The aim of the comparison is to identify parameters for the numerical model which will provide an improved forecast of future observations of the physical system. There are many different methods for data assimilation. In this instance 4D-Variational (4D-Var) data assimilation is considered.

4D-Var data assimilation involves using an approximation for the initial condition, called the analysis vector, of the model in order to form results for comparison with the observations. The analysis vector is found such that it produces the least squares solution between the results from the simulation and the observations taken over the assimilation window. The simulation is continued for a period of time longer than the assimilation window in order to generate a forecast for the physical system. This is how operational weather forecast centers generate weather forecasts.

However errors can affect the results of 4D-Var data assimilation and come from many different sources. For example, model error is introduced through the equations of the model inaccurately simulating the true physical system, and numerical error during the solution of the equations. In this case we are interested in the numerical error and its effects during 4D-Var data assimilation. In order to understand the effects of numerical model error, the linear advection equation is investigated, $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$,

$$u_t(x,t) + u_x(x,t) = 0.$$

Numerical model error is introduced when simulating the linear advection equation through the approximation of the derivatives using finite difference methods. The aim is to understand how the application of different finite dif-

ference methods for the equation affects the accuracy of the outcome from the inverse problem.

Many finite difference schemes have been designed to solve the linear advection equation, such as the Lax-Wendroff and Box Scheme. The dispersive and dissipative effects of these methods become apparent over time through the affect of the numerical methods on the different frequency components of the wave. In this presentation we discuss the effects of the dispersive and dissipative properties of several methods in relation to 4D-Variational data assimilation. Here we consider a shock profile with periodic boundary conditions and consider the accuracy of the resultant analysis vector and its forecast over the assimilation window.

Domain Decomposition for Reaction-Diffusion Systems

Rodrigue Kammogne & Daniel Loghin *(University of Birmingham)*

Domain **D**ecomposition (**DD**) methods have been successfully used to solve elliptic problems , as they are dealing with the problem in a more elegant and efficient way by dividing the domain into subdomains and then obtaining the solution by solving smaller problems on these subdomains. Furthermore **DD**−techniques can incorporate in their implementation not only the physics of the different phenomena associated with the modeling , but also the enhancement of parallel computing. They can be divided into two major categories: with and without overlapping. The most important factor in either case is the ability to solve the interface problem referred as the Steklov-Poincaré. For solving the interface problem there exist two approaches. The first approach,which consists of approximating the interface problem by a sequence of subdomains problem and the second approach, which aims to tackle the interface problem directly. As far as we know none of these have been applied on reaction diffusion systems.
In the past few years reaction diffusion systems have received a strong attention as the have been widely used in biological , chemical and recently in financial modeling. Obtaining a numerical solution for reaction diffusion systems remains a challenging task.
In our presentation we consider the following generic system :

$$\begin{cases} u_t - \Delta u = & f(u) & \text{in } \Omega \\ \mathcal{B}u = & g & \text{on } \partial\Omega \end{cases}$$

where $u = (u_1, u_2)$ and $f \in \mathbb{R}^2$.

We will describe how **DD**−methods can be used to tackle reaction diffusion systems problems in the non-overlapping case. Furthermore by addressing the problem directly on the interface we will present and analyze different **DD**-Preconditioners of the Schur-complement for solving the arising linear system , as this lead to a solution technique independent to the mesh parameter. More precisely , we will exploit the fact that the Steklov-Poincaré operators arising in a non-overlapping **DD**−algorithm are coercive and continuous with respect to Sobolev norms of index 1/2. Finally we will validate the theoretical results on numerical experiments drawn from biological applications.

Improved $T - \psi$ finite element schemes for eddy current problems

Tong Kang & Tao Chen *(Communication University of China)*

The aim of this paper is to propose improved $T - \psi$ finite element schemes for eddy current problems in the three-dimensional bounded domain with a simply-connected conductor. In order to utilize nodal nite elements in space discretization, we decompose the magnetic eld into summation of a vector potential and the gradient of a scalar potential in the conductor; while in the nonconducting domain, we only deal with the gradient of the scalar scalar. As distinguished from the traditional coupled scheme with both vector and scalar potentials solved in a discretizing equation system, the proposed decoupled scheme is presented to solve them at two separate equation systems, which avoids solving a saddle-point equation system like the coupled scheme and leads to an important saving in computational eort. The simulation results and the data comparison of TEAM Workshop Benchmark Problem 7 between the traditional coupled scheme and our decoupled scheme show the validity and eciency of the decoupled one.

Convergence of an implicit algorithm for a finite family of asymptotically quasi-nonexpansive maps

Abdul Rahim Khan, Hafiz Fukhar-ud-din & Muhammad Aqeel Ahmad Khan *(King Fahd University of Petroleum and Minerals)*

The proof of the celebrated Banach contraction principle hinges on "Picard iteration". The principle, on the one hand, itself can be implemented on a computer to approximate fixed point of a contractive map to any required accuracy and on the other hand, it is applicable to a variety of subjects such as partial differential equations, integral equations and image processing. This signifies prime importance of the iterative approximation of fixed points in theoretical numerical analysis.

In this paper, we study weak and strong convergence of a new two-step implicit algorithm for a finite family of asymptotically quasi-nonexpansive maps in a uniformly convex Banach space. The results are proved for a more general implicit iterative scheme under weaker assumptions on the control sequences of parameters. Our results are generalization of several well-known results from the current literature.

Linear rational finite differences and applications

Georges Klein & Jean–Paul Berrut *(University of Fribourg)*

The barycentric rational interpolants introduced by Floater and Hormann in 2007 are "blends" of polynomial interpolants of fixed degree d. In some cases these rational

functions achieve approximations of much higher quality than the classical polynomial interpolants, which, e.g., are ill-conditioned and lead to Runge's phenomenon if the interpolation nodes are equispaced. Besides being good interpolants for such a distribution of nodes, the rational functions are suited for applications as well. We will present linear rational finite difference methods and some of their applications.

Norm Growth and Pseudospectra for PML Discretisations of Open Systems

Jacopo Lanzoni & Timo Betcke *(University College of London)*

A standard tool for the solution of acoustic scattering problems in open systems is the use of perfectly matched layers to cut-off the computational domain. Although the corresponding operator has a bounded inverse for real wavenumbers, it can nevertheless exhibit large norm-growth on the real axis in the neighborhood of complex resonances. In this talk we investigate this norm growth in the neighborhood of eigenvalues of PML discretisations. The suitable tool to do this is to compute generalised pseudospectra of the discretised problem. Since PML discretisations lead to large, sparse matrices we will use reduction techniques to make the pseudospectra computations feasible. We apply this approach to several interesting problems, where resonances are close to the real axis and also study the influence of the PML parameters on the pseudospectra of the discretised problems.

Fractional Matrix Powers

Lijing Lin & Nicholas J. Higham *(University of Manchester)*

The aim of this work is to devise a reliable algorithm for computing A^p for $A \in \mathbb{C}^{n\times n}$ and arbitrary $p \in \mathbb{R}$. The need to compute fractional powers A^p arises in a variety of applications, including Markov chain models in finance and healthcare, fractional differential equations, discrete representations of norms corresponding to finite element discretizations of fractional Sobolev spaces, and the computation of geodesic-midpoints in neural networks. Here, p is an arbitrary real number, not necessarily rational. Often, p is the reciprocal of a positive integer q, in which case $X = A^p = A^{1/q}$ is a qth root of A. Various methods are available for the qth root problem. However, none of these methods is applicable for arbitrary real p. In this work, a new algorithm is developed for computing arbitrary real powers A^p. The algorithm starts with a Schur decomposition, takes k square roots of the triangular factor T, evaluates an $[m/m]$ Padé approximant of $(1-x)^p$ at $I - T^{1/2^k}$, and squares the result k times. The parameters k and m are chosen to minimize the cost subject to achieving double precision accuracy in the evaluation of the Padé approximant, making use of a result that bounds the error in the matrix Padé approximant by the error in the scalar Padé approximant with argument the norm of the matrix. The Padé approximant is evaluated from the continued fraction representation in bottom-up fashion, which is shown to be numerically stable. In the squaring phase the diagonal and first superdiagonal are computed from explicit formulae for $T^{p/2^j}$, yielding increased accuracy. Since the basic algorithm is designed for $p \in (-1, 1)$, a criterion for reducing an arbitrary real p to this range is developed, making use of bounds for the condition number of the A^p problem. How best to compute A^k for a negative integer k is also investigated. In numerical experiments the new algorithm is found to be superior in accuracy and stability to several alternatives, including the use of an eigendecomposition and approaches based on the formula $A^p = \exp(p\log(A))$.

Robust Solution of a BVP arising in Liquid Crystal Modelling

John Mackenzie, Craig Macdonald, Chris Newton & Alison Ramage *(University of Strathclyde)*

In this talk I will discuss the use of an adaptive finite element method to solve a non-linear singularly perturbed boundary value problem which arises from a one-dimensional Q-tensor model of liquid crystals. The adaptive non-uniform mesh is generated by equidistribution of a strictly positive monitor function which is a linear combination of a constant floor and a power of the second derivative of the numerical solution. By an appropriate selection of the monitor function parameters, we show that the accuracy of the computed numerical solution is robust to the size of the singular perturbation parameter and achieves an optimal rate of convergence with respect to the mesh density.

Fast Direct Solvers for Elliptic PDEs

Per-Gunnar Martinsson *(University of Colorado at Boulder)*

That the linear systems of algebraic equations arising upon the discretization of elliptic PDEs can be solved very rapidly is well-known, and many successful iterative solvers with linear complexity have been constructed (multigrid, Krylov methods, etc). More recently, it has been demonstrated that it is also often possible to directly compute an approximate inverse (or LU/Cholesky factorization) to the coefficient matrix in linear or close to linear time. The inverse is computed in a data-sparse format that exploits internal matrix structure such as rank-deficiencies in the off-diagonal blocks.

The talk will focus on methods relying on the *Hierarchically Semi-Separable (HSS)* matrix format to efficiently represent the solution operator to the PDE. This format is less versatile than the more popular $\mathcal{H}$ and $\mathcal{H}^2$ matrix formats, but typically results in very high performance in terms of speed and accuracy when it can be made to work. For problems on 1D domains such as a boundary integral equation (BIE) on a domain in the plane, the adaptation of the HSS format is straight-forward, and problems in higher dimensions can be handled via recursive domain decomposition techniques that reduce the dimensionality of the domain on which the compressed operator acts.

The talk will describe numerical examples in both two and

three dimensions. Variable coefficient problems are handled via accelerated nested dissection methods, while constant coefficient problems are solved via the corresponding boundary integral equation formulations.

The relation between two algorithms for enclosing matrix eigenvalues

Shinya Miyajima *(Gifu University)*

In this talk, we are concerned with accuracy of computed eigenvalues for

$$Ax = \lambda x, \qquad A \in \mathbb{C}^{n\times n}, \quad \lambda \in \mathbb{C} \quad x \in \mathbb{C}^n, \qquad (1)$$

where λ is an eigenvalue and x is an eigenvector corresponding to λ.

There are several algorithms for enclosing eigenvalues in (1), *e.g.,* [2, 3]. Especially we consider the algorithms for enclosing all eigenvalues which is applicable even when A is not Hermitian. Such an algorithm has been proposed in [2, Algorithm 2], which is based on the following theorem:

Theorem 1 (Oishi [2]) Assume as a result of numerical computation, we have an $n \times n$ complex diagonal matrix $\tilde{D}$ and an $n \times n$ complex matrix $\tilde{X}$ such that $A\tilde{X} \approx \tilde{X}\tilde{D}$ follows approximately. Let $\tilde{\lambda}_i$, $i = 1, \ldots, n$ and $\| \cdot \|$ be the (i, i) element of $\tilde{D}$ and a norm satisfying $\| FG \| \leq \| F \| \| G$ for $F, G \in \mathbb{C}^{n\times n}$, respectively. Denote the $n \times n$ identity matrix by I. For an arbitrary $n \times n$ complex matrix Y, define $n \times n$ complex matrices R and S as $R := YA\tilde{X} - \tilde{D}, \quad S := Y\tilde{X} - I$. Then it holds that $\min_{\leq i\leq n} |\lambda - \tilde{\lambda}_i| \leq \epsilon_o, \ \epsilon_o := \| R \| + \| A \| \| S \|$.

On the other hand, a theorem has been presented in [1] for enclosing all eigenvalues in the generalized eigenvalue problem

$$Ax = \lambda Bx, \qquad A, B \in \mathbb{C}^{n\times n}, \quad \lambda \in \mathbb{C} \quad x \in \mathbb{C}^n \qquad (2)$$

This theorem is also applicable even when A is not Hermitian. We can utilize this theorem for enclosing all eigenvalues in the standard eigenvalue problem (1) by substituting $B = I$ into (2). Then we obtain the following theorem:

Theorem 2 (Miyajima [1]) *Let* $\tilde{D}$, $\tilde{X}$, $\tilde{\lambda}_i, \| \cdot \|, I, Y$ and S be defined as in Theorem 1. Define an $n \times n$ complex matrix T as $T := Y(A\tilde{X} - \tilde{X}\tilde{D}$. If $\| S \| < 1$, then $\tilde{X}$ and Y are nonsingular, and it follows that $\min_{1\leq i\leq n} |\lambda - \tilde{\lambda}_i| \leq \epsilon_m, \epsilon_m := \dfrac{\| T \|}{1 - \| S \|}$.

The purpose of this talk is to present a theorem showing that $\epsilon_o \geq \epsilon_m$ holds if $\max_{1\leq i\leq n} |\tilde{\lambda}_i| + \epsilon_o \leq \| A \|$ and $\| S \| < 1$ hold. We discuss the validity of these assumptions, and report some numerical results for confirming that the presented theorem is true and showing that these assumptions follow in many cases.

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An efficient finite volume method applied to flow in heterogeneous porous media

Tim Moroney, Ben Cumming, Kevin Burrage & Ian Turner *(Queensland University of Technology)*

We present a finite volume method for efficiently solving Richards' equation in heterogeneous porous media. The spatial discretisation of the governing partial differential equation naturally handles heterogeneous media on unstructured meshes by allowing discontinuities in conserved quantities, such as moisture content, at the interface between media. At each node, a pair of algebraic and differential equations is produced, and the resulting system is solved efficiently using backward differentiation formulae. The inclusion of the algebraic equations results in excellent mass conservation in the computed solution, and an appropriately tailored preconditioner largely mitigates the additional cost.

This formulation makes extensive use of basic dense and sparse linear algebra operations, making it an excellent candidate for graphics processing unit (GPU) acceleration. We show how C++ templates allow for the same high-level code to be run on either CPUs or GPUs, with technologies such as CUDA, MPI and openMP used to extract maximum performance from the machine.

Results are exhibited that show how this formulation produces accurate and efficient solutions to problems in heterogeneous media. Timings for multicore CPU and GPU runs demonstrate that this formulation is amenable to effective GPU acceleration.

Arithmetic and communication minimizing algorithms for the symmetric eigenvalue problem and the singular value decomposition

Yuji Nakatsukasa *(University of California, Davis)*

The total cost of an algorithm is a combination of its arithmetic cost and communication cost. Recently there has been considerable progress in the development of linear algebra algorithms that minimize communication (e.g., [**?**]). However, the reduction in communication cost sometimes comes at the expense of significantly more arithmetic. This includes the recently-proposed communication-minimizing algorithms [**?**] for computing the symmetric eigenvalue decomposition and the singular value decomposition (SVD). These algorithms also suffer from potential instability.

In this talk I will describe algorithms for these two decompositions that minimize both communication and arithmetic, up to a constant factor smaller than 3. Both algorithms are based on a QR-based algorithm [**?**] for computing the polar decomposition. The essential cost for each of these algorithms is in performing QR decompositions

of the form $\begin{bmatrix} X \\ I \end{bmatrix} = QR$, of which we require no more than 6 for the symmetric eigendecomposition, and 12 for the SVD. I will establish backward stability of these algorithms under mild assumptions. Preliminary numerical experiments demonstrate their efficiency.

Optimal state and parameter estimation using a hybrid data assimilation scheme

N K Nichols P J Smith and S L Dance *(University of Reading)*

A numerical model can never completely describe the complex physical processes underlying the behaviour of a real world dynamical system. State of the art computational models are becom- ing increasingly sophisticated, but in practice these models suffer from uncertainty in their initial conditions and parameters. Mathematical techniques for combining observational data with prior model predictions, known as data assimilation techniques, can be used to construct accurate esti- mates of the initial conditions and parameters in the model and hence improve the ability of the model to predict the true system state. Under certain statistical assumptions on the errors in the prior estimates, the solution to the assimilation problem yields the optimal (maximum a posteriori likelihood) estimate of the true state of the system. A key diffculty in the construction of a data assimilation scheme is specification of the prior error covariances. These covariances play an important role in the filtering and spreading of observational data; however, propagating the background error covariance matrix is computationally expensive. Here we combine ideas from 3D variational assimilation methods and extended Kalman filter tech- niques to produce a new hybrid assimilation scheme that provides a ow dependent approximation to the state-parameter cross covariances without explicitly propagating the full system covariance matrix. This method has been tested in several linear and nonlinear dynamical models, success- fully recovering the the initial states and true parameter values to good accuracy, even with noisy observations. The new technique has also been applied to a simplified model of coastal and estuarine sediment transport to deliver estimates of uncertain morphodynamic parameters with excellent results. Such a system can be used to improve ood forecasting, with clear social and economic bene

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Theoretical analysis of Sinc-collocation methods for weakly singular Volterra integral equations of the second kind

Tomoaki Okayama, Takayasu Matsuo & Masaaki Sugihara *(Hitotsubashi University)*

We are concerned with Volterra integral equations of the second kind of the form

$$u(t) - \int_a^t \frac{k(t,s)}{(t-s)^p} u(s)\,\mathrm{d}s = g(t), \quad a \le t \le b, \qquad (1)$$

where g and k are given smooth functions, p is a constant with $0 < p < 1$, and u is a solution to be determined. The equations have a weakly singular kernel $(t-s)^{-p}$, called the Abel kernel, which diverges at $s = t$. In addition, due to the singularity of the kernel, the solution u may have a derivative singularity at the endpoint $t = a$ [1]. Because of these two singularities, it is not an easy task to construct a high order numerical scheme.

Sinc-collocation methods, which have been developed by Riley [2] and Mori et al. [3], seem successful for the equation (1) in the sense that the resulting schemes can achieve *exponential convergence*. Riley [2] has estimated the error of his numerical solution u_N as

$$\max_{a\le t\le b} |u(t) - u_N(t)| \le C\|A_N^{-1}\|_\infty \sqrt{N} \log N\, \mathrm{e}^{-\sqrt{\pi d(1-p)N}} \qquad (2)$$

where A_N denotes a coefficient matrix of the resulting linear equation, and d is a parameter that indicates the regularity of the solution u. It has been noted that $\|A_N^{-1}\| \le 4$ for N in a "practical range" if the interval $b - a$ is "sufficiently small"[2]. Afterward, Mori et al. [3] have improved the scheme, and estimated the error of the numerical solution as

$$\max_{a\le t\le b} |u(t) - u_N(t)| \le C\|B_N^{-1}\|_\infty \log N\, \mathrm{e}^{-\pi dN/\log(2dN/p)} \qquad (3)$$

where B_N is also a coefficient matrix. This estimate also suggests that the scheme can achieve exponential convergence, if $\|B_N^{-1}\|_\infty$ do not increase rapidly. This has also been confirmed by some numerical experiments.

One of the purposes of this study is to prove exponential convergence of the two schemes in a rigorous sense. This is done by showing

$$\|A_N^{-1}\|_\infty \le C_1 \log N, \qquad \|B_N^{-1}\|_\infty \le C_2 \log N, \qquad (4)$$

for *all* sufficiently large N, and for *any length* of the interval $b - a$. The existence of the inverse matrices A_N^{-1} and B_N^{-1} is also proved. Another purpose of this study is to estimate the parameter d, which is indispensable for implementing the schemes and affects the convergence rate as estimated above. This is done by applying the technique established for Fredholm integral equations [4].

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Using data assimilation within a moving mesh approach to ice sheet modelling

Dale Partridge, Mike Baines & Nancy Nichols *(University of Reading)*

Computational studies of glaciers are particularly challenging to the modeller. Although ice sheet models are well-established, prediction of profiles are generally infeasible analytically and difficult to achieve numerically. Many fixed grid methods lose large amounts of information due to the sparse nature of grid points, necessitated by the large spatial scales ice sheets can cover. A moving mesh approach to numerical modelling of glaciers has been proposed, based on the shallow ice approximation equations, where the mesh is driven by relative mass conservation. This approach is being tested against benchmark experiments set up to compare different models.

We apply the techniques of data assimilation, combining the model with observations to improve our estimate of the state of the system in order to correct the model and overcome some of the deficiancies that arise under moving mesh methods. Due to the nature of the methods, the mesh points themselves are variables in the model which can be manipulated bu correctly applied assimilation.

Dual Lumping of Isogeometric Finite Element Schemes using Petrov-Galerkin Techniques

Mark Payne & Dugald Duncan *(Heriot-Watt University)*

The isogeometric finite element method, introduced by Hughes et al. 2005, uses non-uniform rational B-splines (NURBS) as a basis for test and trial functions. The strengths of using NURBS is the fact that they have excellent approximation properties and can easily be produced via the Cox-de Boor recursion formula. NURBS however, except for crude row sum mass lumping techniques, cannot easily produce diagonal mass matrices for hyperbolic problems. In particular, the standard spectral element approach cannot be used due to their non-negative nature. One idea is to use a Petrov-Galerkin approach, producing an orthogonal dual basis which is then used as the test functions as discussed in Cottrell et al. 2009. Common examples of dual basis are discontinuous and therefore integration by parts cannot be used. We adapt the technique, using a smooth dual basis that is orthogonal to the NURBS basis only in respect to an approximate quadrature. This allows us to intergrate by parts with the additional advantage to choose the test functions suitably to optimize convergence and accuracy. We apply this approach to the acoustic wave equation and compare it with the spectral element method and the row sum mass lumping method.

DQM Time-DQM Space Solution of Hyperbolic Telegraph Equation

Bengisen Pekmen & Munevver Tezer-Sezgin *(Atilim Universit)*

Differential Quadrature Method (DQM) is proposed both in space and time directions for the numerical solutions of one- and two-dimensional hyperbolic telegraph equations. The equation in two-space dimension is $u_{tt}+2\alpha u_t+\beta^2 u - u_{xx}-u_{yy}=f(x,y,t),\ 0\le x,y,\le 1,\ t\ge 0$ where $\alpha\ge\beta>0$, and it is subjected to appropriate initial and boundary conditions. The DQM formulation of this equation gives a main system $[B]\{u\}=\{knowns\}$ of which B is the coefficient matrix consisting of the known DQM weigthing coefficients, and the known vector contains $f(x_i,y_j,t_l)$ as entries. Both the initial condition $u(x,0)$ and Dirichlet boundary conditions are inserted to the system directly, reducing the size and the computational cost. The initial condition $u_t(x,0)$ and Neumann boundary conditions are discretized by using DQM and added to the main system resulting an overdetermined system.

For the solution, the least squares method or QR factorization is used. The solvability of the DQM resulting overdetermined system of equations is related with the column rank of the coefficient matrix. When the initial/or Neumann type boundary conditions are discretized using DQM, and added to the system, the row size is certainly greater than the column size which makes the system overdetermined. The small number of grid points especially in time direction provides a full column rank coefficient matrix. This is one of the main advantage of DQM method in using for the time direction which allows us to be able to use large time increment Δt.

Both polynomial based differential quadrature (PDQ) and Fourier based differential quadrature (FDQ) are used in space directions whereas PDQ is made use of in time direction. Numerical solution is obtained by using Gauss-Chebyshev-Lobatto points in space intervals and equally spaced points for the time interval. DQM in time direction gives the solution directly at a required time level or steady-state without the need of iteration, and it is stable even large Δt is used. The computations are carried for several one- and two-dimensional telegraph equations with Dirichlet and/or Neumann boundary conditions. DQM also has the advantage of giving very good accuracy with considerably small number of discretization points.

Finite elements on pyramids

Joel Phillips *(University College London)*

The differing strengths of tetrahedral and hexahedral finite elements mean that it is sometimes desirable to combine both within the same method. A mesh that contains both tetrahedral and hexahedra will, in general, need quadrilateral-based pyramids to act as “glue” between them; so, if we are to build conforming finite element methods using such a mesh, we need to be able to construct pyramidal finite elements.

In this talk, I will give a brief history of attempts to construct pyramidal finite elements and present our construction of a family of pyramidal analogues to Nedelec’s

elements. These are arbitrarily high order elements for each of the spaces of the de Rham complex which are compatible with tetrahedral and hexahedral elements through their triangular and quadrilateral faces. They satisfy the commuting diagram property necessary to build stable approximations to mixed problems.

I will also prove the surprising result that the approximation space for a pyramidal element cannot be composed only of polynomials. We will see that this means that the standard analysis of the effects of numerical integration on finite elements is inapplicable to pyramidal elements. I will give some insight into how this problem is resolved and then present some numerical examples.

The augmented Lagrangian method with bounds on the dual variables

M.J.D. Powell *(University of Cambridge)*

Let some or all of the constraints of an optimization calculation be treated by an augmented Lagrangian method, the Lagrangian being minimized by the primal variables for each choice of the dual variables (Lagrange multiplier estimates). Then usually the dual variables are optimal when the resultant least value of the Lagrangian takes its maximum value, but, if the given constraints are inconsistent, then this maximum value and some corresponding values of the dual variables may become infinite. Failures of this kind can be avoided by imposing prescribed bounds on the dual variables. Let these bounds be active at the end of the calculation. Then we find, in several situations, that the final values of the primal variables solve a problem where some of the original constraints are replaced by L_1 penalty terms, as in work of P.E. Gill and D.P. Robinson. An interesting application of this technique is described, developed by D.W. Wood, A.A. Groenwold and L.F.P. Etman, for Sequential Approximate Optimization Algorithms that have huge numbers of variables.

Algorithm and error bounds for piecewise linear approximation on anisotropic triangulations

A.F. Rabarison & O. Davydov *(University of Strathclyde)*

Given a square domain $\Omega \subset \mathbb{R}^2$ and a convex function $f \in C^2(\Omega)$, we propose an algorithm for generating a sequence of anisotropic triangulations $\{\mathcal{T}_N : \#(\mathcal{T}_N) \leq N, N \geq N_0\}$ of Ω. For any $p \in [1, \infty)$, the resulting piecewise linear interpolant f_N to f over the triangulation $\mathcal{T}_N$ satisfies the asymptotic estimations

$$\limsup_{N\to\infty} N\|f - f_N\|_{L^p(\Omega)} \leq \left(\int_\Omega K_{f,p}(z)^q \mathrm{d}z\right)^{1/q}, \quad (10)$$

$$\limsup_{N\to\infty} N^{\frac{1}{2}}|f - f_N|_{W^1_p(\Omega)} \lesssim \left(\int_\Omega K_{f,p}(z)^q \mathbb{D}z\right)^{\frac{1}{2}} \left(\int_\Omega |\det H_f(z)|^{\frac{q}{4}} \|H_f(z)\|_2^{\frac{p}{2}} \mathbb{D}z\right)^{\frac{1}{p}} (11)$$

where $1/q = 1 + 1/p$, $H_f(z)$ denotes the Hessian matrix of f at $z \in \Omega$, whereas

$$K_{f,p}(z) := \inf_{|T|=1} \|\pi_z - I_T\pi_z\|_{L^p(T)}$$

$$\pi_z(x, y) = \frac{1}{2}\frac{\partial^2 f(z)}{\partial x^2}x^2 + \frac{\partial^2 f(z)}{\partial x \partial y}xy + \frac{1}{2}\frac{\partial^2 f(z)}{\partial y^2}y^2,$$

and $I_T\pi$ is the linear interpolation polynomial of π over the triangle T. It is known [2] that the estimation (10) cannot be improved on any sequence of triangulations $\mathcal{T}_N$ such that $\sup_{T\in\mathcal{T}_N} \mathrm{diam}(T) \lesssim N^{-1/2}$. Previous constructions do not satisfy (11), with $|f - f_N|_{W^1_p(\Omega)}$ possibly unbounded as $N \to \infty$.

Hirota's bilinear method and the ε–algorithm

M Redivo-Zaglia & C. Brezinski, *(University of Padova)*

Hirota's bilinear method [2] can be quite useful in the solution of nonlinear differential and difference equations. In this talk, we show how this method can lead to a proof that the ε–algorithm of Wynn [5] implements the Shanks' sequence transformation [3, 4] and, reciprocally, that the quantities it computes are expressed as ratios of Hankel determinants as given by Shanks. New identities between the quantities involved in Hirota's method are obtained. Then, the same bunch of results is showed to hold also for the confluent form of the ε–algorithm. Its relation to the Lotka–Volterra equation allows to express the solution of this equation under a closed form. The same technique can be also used for obtaining a multistep extension of the ε–algorithm [1].

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Towards Exascale Computing: Multilevel Methods and Flow Solvers for Millions of Cores

Ulrich Ruede *(University of Erlangen-Nürnberg)*

This presentation will report on experiences implementing PDE solvers on Peta-Scale computers, such as the 290000 core IBM Blue Gene system in the Jülich Supercomputing Center. The talk will have two parts, the first one presenting the Hierarchical Hybrid Grid (HHG) method. HHG is a prototype parallel multigrid algorithm that has

been used to solve FE systems with up to a trillion (10^{12}) degrees of freedom arising form a tetrahedral FE mesh. Excellent scalability and a good absolute efficiency are achieved by a using a matrix-free data structure and a carefully optimized implementation. The second part of the talk will present a brief overview of our work on simulating complex flow phenomena. This will include work on a parallel fluid-structure-interaction technique with many moving rigid objects that are embedded in the flow. Fully resolved geometric representations of each particle are used in a massively parallel simulation of particle-ladden flows. The talk will conclude with some remarks on the challenges that the developers of numerical algorithms will be facing on the path to exascale in the coming years.

Numerical Solution of Fully Nonlinear Elliptic PDEs with a Modified Argyris Element

Abid Saeed & Oleg Davydov *(University of Strathclyde)*

We discuss an implementation of Böhmer's finite element method for fully nonlinear elliptic partial differential equations. In this method the nonlinear problem is solved iteratively by a Newton scheme yielding a sequence of linear elliptic equations for good initial guess. Discretisation is done by modified Argyris finite elements that admit a stable splitting. Implementation is done using the Bernstein-Bézier techniques for modified Argyris elements. We consider the Dirichlet problems for several fully nonlinear equations including *Monge-Ampère equation* over convex polygonal domains. The numerical results for several test problems illustrate the expected rate of convergence of the scheme.

Energy Minimizing Coarse Spaces with Functional Constraints

Robert Scheichl, Panayot Vassilevski & Ludmil Zikatanov *(University of Bath)*

We will report on the construction of energy minimizing coarse spaces for the robust approximation of PDE solutions in the case of strongly varying and high contrast coefficients. The spaces are built by patching together solutions to appropriate local saddle point problems or eigenproblems. They can be used either in two-level Schwarz methods or directly to approximate the PDE solution on meshes that do not resolve the coefficient variation. We first set an abstract framework for such constructions, and then we give two examples of constructing the coarse space and a stable interpolation operator for the two level Schwarz method. The stability and approximation bounds of the constructed interpolant are in a weighted norm and are independent of the variations in the coefficients. Part of this work was done jointly with Victorita Dolean (University of Nice Sophia–Antipolis), Frederic Nataf and Nicole Spillane (both University of Paris VI).

Higher order variational time discretizations for nonlinear systems of ordinary differential equations

Friedhelm Schieweck & Gunar Matthies *(University of Magdeburg)*

We discuss different time discretizations of variational type applied to a nonlinear system of ordinary differential equations which is typically generated by a semi-discretization in space of a given nonlinear parabolic partial differential equation like, for instance, the non-stationary Burgers equation.

Among these methods we compare the known continuous Galerkin-Petrov and the discontinuous Galerkin method with time polynomial ansatz functions of order k (cGP(k)- and dG(k)-method) with respect to accuracy, stability and computational costs. Moreover, we propose two new extended methods (cGP-C1(k+1)- and dG-C0(k+1)-method) which have on the one hand a one higher degree of ansatz functions and accuracy, the same stability properties and on the other hand the same computational costs as the original methods. We prove A-stability for the cGP-methods and strong A-stability for the dG-methods.

We present optimal error estimates and the close relationship between the original and extended methods which prove as a byproduct the super-convergence of the original methods cGP(2) and dG(1) in the endpoints of all discrete time intervals. Finally, we present first numerical results for the non-stationary Burgers equation in one space dimension.

A Lax-Wendroff type numerical method for a fractional advection diffusion equation

Ercília Sousa *(Coimbra University)*

Recently, many transport problems, involving diffusion, have been formulated on fractional differential equations. Fractional derivatives are non-local opposed to the local behaviour of the integer derivatives and they are used to model a phenomenon called anomalous diffusion, which can be subdiffusion or supersiffusion. In this work, we are interested in the superdiffusion.

A one dimensional fractional advection diffusion model is considered, where the usual second-order derivative gives place to a fractional derivative of order α, with $1 < \alpha \leq 2$. The fractional derivative is defined by the Riemann-Liouville operator, which is an integral operator. We propose an explicit difference method which is second order accurate. Consistency and stability of the method are examined and numerical tests are presented.

A new splitting method for mean curvature-based variational image denoising

Li Sun & Ke Chen *(University of Liverpool)*

Denoising perhaps is one of the most fundamental tasks in image processing. It has been deeply investigated for many years and many excellent results have been obtained by using Total Variation (TV) based L1-model. While the model can preserve important features such as sharp edges and contours, for smooth images however, the TV model

produces undesirable staircasing effect. In order to remedy this drawback, many researchers have turned to higher order models. The particular model using mean curvature as a regulariser, shown to be effective for general denoising by Zhu and Chan 2006 (W. Zhu and T. F. Chan, "Image Denoising Using Mean Curvature", preprint, http://www.math.nyu.edu/ wzhu/, 2006); Brito and Chen 2010 (Carlos Brito and Ke Chen, "Multigrid Algorithm for High Order Denoising", SIAM Journal on Imaging Sciences, Vol 3 (3), pp.363-389, 2010), is studied in this work and we have proposed an efficient and robust iterative method for its numerical solution.
Due to strong nonlinearity, the resulting Euler-Lagrange partial differential equation is of fourth order and convergence is extremely slow with gradient descents [Zhu and Chan 2006]. The stabilisation method adopted by Carlos Brito and Ke Chen 2010 was a major improvement but it has to severely regularise the nonlinearity. After first applying the 2-level splitting method of Tai 2011 (Xue-Cheng Tai, J. Hahn, and G. J. Chung, "A Fast Algorithm for Euler's Elastica Model Using Augmented Lagrangian Method", SIAM Journal on Imaging Sciences, Vol 4, pp. 313-344 , 2011), we found that the restored quality is not as good as the original curvature model although the resulting numerical scheme is indeed fast. To reduce the level of approximations, we consider one-level splitting method in this work. We derived and implemented the precise boundary conditions (BCs) using staggered grids and locally coupled iterative solvers instead of using the usual Neumann BCs which are found not suitable. It turns out that both the Newton method and a Fixed point method are convergent, and they are suitable for a nonlinear multigrid method. Numerical results can show that our model can deliver better quality of restoration than the previous fast methods, by using less regularisation of the nonlinearity than Brito and Chen 2010.

iGen: a program for the automated generation of reduced-dimension models

Dan F. Tang *(Manchester University)*

In this presentation I will describe a novel approach to the generation of reduced dimension models from high-dimensional models. The approach involves expressing the high-dimensional model as a computer program written in C++. The source code of this program is then fed into a newly developed computer program called iGen. iGen analyses the structure of the source code, represents sections of code as multivariate polynomials with constant error bounds and approximates these polynomials with lower-order polynomials. From the analysis, iGen derives a reduced-dimension model that closely approximates the original, while reporting bounds on the error introduced by any approximations. I will describe the application of iGen to a number of increasingly complex physical systems and show that iGen has the ability to generate reduced models that execute typically orders of magnitude faster than the underlying, high-dimensional models from which they are derived.

Multilevel Monte Carlo for highly heterogeneous media

Aretha Teckentrup, J. Charrier, K.A. Cliffe, M.B. Giles and R. Scheichl *(University of Bath)*

The quantification of uncertainty in groundwater flow plays a central role in the safety assessment of radioactive waste disposal and of CO2 capture and storage underground. Stochastic modelling of data uncertainties in the rock permeabilities lead to elliptic PDEs with random coefficients. Because of the typically large variances and short correlation lengths in groundwater flow applications, methods based on truncated Karhunen-Loeve expansions are only of limited use and Monte Carlo type methods are still most commonly used in practice. To overcome the notoriously slow convergence of conventional Monte Carlo, we formulate and implement a novel variance reduction technique based on hierarchies of spatial grids/models. This multilevel Monte Carlo method was first introduced for high-dimensional quadrature by Heinrich (2001) and for stochastic ODEs in mathematical finance by Giles (2007). We will demonstrate theoretically and practically on a typical model problem the significant gains with respect to conventional Monte Carlo that are possible with this new approach, leading (in the best case) to an asymptotic computational cost that is proportional to the cost of solving one deterministic PDE to the same accuracy.

MHD flow and heat transfer between parallel plates with Navier-slip wall condition

Münevver Tezer-Sezgin & Önder Türk *(Middle East Technical University)*

The magnetohydrodynamic (MHD) flow of a dusty fluid with heat transfer between parallel plates, in which the fluid has temperature dependent thermal conductivity and viscosity, is solved by using Chebyshev spectral collocation method. An external uniform magnetic field is applied perpendicular to the plates, and the fluid is driven by a constant pressure gradient G. The plates are electrically insulated and kept at constant temperatures. The dust particles are assumed to be spherical in shape and uniformly distributed throughout the fluid. The governing equations are given in terms of fluid velocity and temperature u, T, and particles velocity and temperature u_p, T_p, respectively, as

$$
\begin{aligned}
&Re\frac{\partial u}{\partial t} = Re\ G + \frac{\partial}{\partial y}\left[\mu(T)\frac{\partial u}{\partial y}\right] - Ha^2 u - R(u-u_p),\\
&\frac{\partial u_p}{\partial t} = \frac{1}{Re\ g}(u-u_p),\\
&Re\frac{\partial T}{\partial t} = \frac{1}{Pr}\frac{\partial}{\partial y}\left(\kappa(T)\frac{\partial T}{\partial y}\right) + Ec\ \mu(T)\left(\frac{\partial u}{\partial y}\right)^2\\
&\qquad +Ec\ Ha^2\ u^2 + \tfrac{2R}{3Pr}(T_p - T),\\
&\frac{\partial T_p}{\partial t} = -L(T_p - T),
\end{aligned}
$$

where $0 \le y \le 1,\ t > 0$, and $\mu(T) = e^{-aT}$, $\kappa(T) = e^{bT}$.

Navier-slip condition is imposed for both the fluid and par-

ticle velocities on the plates which constitutes the proportion of velocities to the tangential viscous stresses with a parameter. The Chebyshev spectral method allows one to be able to use considerably small number of Chebyshev-Gauss-Lobatto space points clustered through ends. Implicit backward difference is used for the temperature derivatives which is unconditionally stable and uses quite large time steps. This makes the whole solution procedure computationally cheap and efficient. The effect of the wall slip parameter, viscosity $\mu(T)$ and thermal conductivity $\kappa(T)$ variations, and the uniform magnetic field for both the fluid and the dust particles is studied. It is found that the velocities of both fluid and dust particles decrease as Hartmann number Ha is increased, when Reynolds number Re, Prandtl number Pr, Eckert number Ec, particle concentration parameter R are kept fixed. An increase in the Navier-slip parameter causes increases in the magnitude of velocities of dust particles and the fluid. The effect of viscosity parameter variation is more stressed on the velocity profiles than the temperature. Variations (especially increase) in the thermal conductivity parameter result in temperature variations in non-linear manner, but the velocities are not much affected.

Multiscale analysis in Sobolev Spaces on bounded domains with restricted interpola- tion points

Alex Townsend *(University of Oxford)*

A multiscale scheme is studied for the approximation of Sobolev functions on bounded domains with restricted data sites. Our method employs compactly supported radial basis functions with centers at scattered data sites restricted at each level to ensure the support of the interpolant is contained within the domain. The multiscale approximation is constructed by successive residual corrections with each level using a support radii appropriate to capture dfferent scales. Important steps in the proof of the convergence theorem for the scheme will be shown with an improved rate if the target function and its derivatives vanishes on the boundary. We will also present some numerical examples of the scheme which reinforce the theory. This analysis is hoped to be a first step towards understanding domain boundary effects for radial basis function interpolation and to improve the numerical solution of partial differential equations on bounded domains.

Chebyshev spectral collocation method for unsteady MHD flow and heat transfer between parallel plates

Önder Türk *(Middle East Technical University)*

The magnetohydrodynamic (MHD) flow with heat transfer of a Newtonian, incompressible fluid which has temperature dependent viscosity is solved between parallel plates. An external uniform magnetic field is applied perpendicular to the plates, and the fluid is driven by a constant pressure gradient G. The movement of the upper plate with a constant velocity Ru, and the convection action in terms of inflow/outflow through plates are also considered. The plates are electrically insulated. The governing equations are written in non-dimensional form in terms of velocity u, temperature T

$$\frac{\partial u}{\partial t} + Rv\frac{\partial u}{\partial y} = G + \frac{\partial}{\partial y}\left[\mu(T)\frac{\partial u}{\partial y}\right] - Ha^2 u,$$

$$\frac{\partial T}{\partial t} + Rv\frac{\partial T}{\partial y} = \frac{1}{Pr}\frac{\partial^2 T}{\partial y^2} + Ec\ \mu(T)\left(\frac{\partial u}{\partial y}\right)^2 + Ec\ Ha^2\ u^2, \tag{12}$$

where $-1 \le y \le 1,\ t > 0$ and $\mu(T) = e^{-aT}$ is the variable viscosity.

These coupled nonlinear partial differential equations together with convenient boundary conditions are solved numerically. The Chebyshev spectral collocation method is used for space derivatives whereas implicit backward difference is made use of for temporal derivatives which is unconditionally stable and does not need too small time step. The Chebyshev spectral method allows one to be able to use considerably small number of clustered Chebyshev-Gauss-Lobatto points in space direction. Also, it is easy and practical to obtain higher order derivative approximations of the solution by using only multiplications of Chebyshev differentiation matrices. This makes the whole procedure computationally cheap and efficient. Numerical results are visualized in terms of velocity and temperature of the fluid for several values of Hartmann number (Ha) and viscosity parameter (a) for depicting the influences on the flow and temperature. Results for the velocity and temperature field are obtained for several values of Hartmann number, viscosity parameter, upper plate velocity (Ru), inflow/outflow parameters (Rv) when Prandtl number $Pr = 1$, Eckert number $Ec = 0.2$ and $G = 5$ are taken. The effects of variable (temperature dependent) viscosity and applied magnetic field are deeply examined. The fluid starts with the interaction of pressure gradient and the externally applied magnetic field. An increase in viscosity parameter a causes increase in the magnitudes of both velocity and temperature. But as Ha increases, flow is decreased sharply, temperature also drops but settles down for $Ha \ge 10$. As Ha is increased boundary layers are formed near the insulating plates which is the expected behavior of MHD flow. As time progresses both velocity and temperature increase and reach steady-state before $t = 5$. Drop in the magnitudes of velocity and temperature is also observed in the presence of convection terms (inflow/outflow through plates). With the movement of the upper plate the temperature is not affected as much as the velocity. The use of Chebyshev spectral method when it is combined with the unconditionally stable backward difference time integration, enables one to obtain very good accuracy with considerably small number of collocation points, and quite large time steps. This makes the solution procedure computationally efficient.

Distributing Points in a Triangle using Optimal Transport Techniques

Jan Van lent & Chris Budd *(University of the West of England)*

Generating point distributions and meshes for a given do-

main is an important problem in numerical analysis. The one-dimensional problem of generating points in an interval that are suitable for interpolation and quadrature is fairly well understood. Chebyshev points, for example, perform very well. However, already for a simple two-dimensional domain such as a triangle, generating good point distributions is still an active research topic. In this talk I will discuss techniques for generating points and meshes based on numerical methods for the Monge-Kantorovich optimal transport problem. I will illustrate how these techniques can be used for triangular domains.

Numerical analysis of two-phase granular flows at low Mach numbers

C. Varsakelis & M. V. Papalexandris *(Université Catholique de Louvain)*

In this talk we present an algorithm for the numerical treatment of a continuum two-velocity, two-pressure model for two-phase granular flows. The proposed method belongs to the class of fractional-step methods and employs a generalized projection scheme for the momentum equation of each phase. It is further able to deal with strong spatial gradients and moving interfaces; both common characteristics of the flows of interest. The talk is concluded with the presentation of numerical simulations which illustrate the accuracy and robustness of the proposed algorithm.

A Posteriori Error Analysis for a Quasicontinuum Method

Hao Wang & Christoph Ortner *(University of Oxford)*

The Quasicontinuum (QC) Method is a method for modeling an atomistic system by coupling an atomistic model and a continuum approximation together. The atomistic model is used in the region where large deformation such as fracture happens so that the full atomistic detail is retained while a continuum model is used in the rest of the material so that the computational work is significantly reduced. In this work, we have given the a posteriori error analysis for Consistent Atomistic/Continuum Coupling QC method, which was developed recently and is an consistent and efficient coupling method in one and two dimensional atomistic system with two body interaction potentials. This method is also promising in the extension to three dimensional systems and general interaction potentials. There are only a few researches on the a posteriori error analysis of QC methods. In our work, we use the negative-norm residual analysis to derive an efficient estimator of the global error of the deformation in a Sobolev norm. We also give the estimator of the error of the energy, i.e, the difference between the energy under the computed deformation and that under the real deformation. An adaptive mesh refinement strategy is developed based on these error estimators and is illustrated in some numerical experiments. A comparison is also made between the efficiency of this refinement strategy and that of an a priori quasi-optimal mesh generation strategy developed in another literature.

Novel numerical methods for nonlinear time-space fractional diffusion equations in two dimensions

Qianqian Yang, Tim Moroney, Kevin Burrage, Ian Turner & Fawang Liu *(Queensland University of Technology)*

In this talk, nonlinear time-space fractional diffusion equations in two dimensions (NTSFDE-2D) are considered. The NTSFDE-2D is obtained from the standard diffusion equation by replacing the first-order time derivative with the Caputo fractional derivative, and the second order space derivatives with the fractional Laplacian. Using the matrix transfer technique proposed by Ilic, Liu, Turner, and Anh (*Fractional Calculus and Applied Analysis*, 9, 333-349, 2006), the NTSFDE-2D is transformed into a time fractional differential system, where $\mathbf{A}$ is the approximate matrix representation of the standard Laplacian. Traditional approximation of the fractional Laplacian requires diagonalisation of $\mathbf{A}$, which is very time-consuming for large matrices. The novelty of our proposed numerical scheme is that, using the finite difference method to approximate the Caputo time fractional derivative, the solution of the NTSFDE-2D is written in terms of a matrix function vector product at each time step. We use the finite volume method over unstructured meshes to generate the matrix $\mathbf{A}$, and the Lanczos method to approximate the matrix function vector product. Numerical results are presented to verify the accuracy and efficiency of the proposed numerical solution strategies.

C^1 Piecewise Quadratic Hierarchical Bases

Wee Ping Yeo & Oleg Davydov *(University of Strathclyde)*

On general triangulations of arbitrary polygonal domains $\Omega \subset \mathbb{R}^2$, we construct C^1 continuous piecewise quadratic hierarchical bases which generate Riesz bases for the Sobolev spaces $H^s(\Omega)$, with $s \in (1, \frac{5}{2})$. The nested approximation spaces used in our construction are the spaces of C^1 piecewise quadratic polynomials on combination of Powell-Sabin-6 and Powell-Sabin-12 triangulations, the same spline spaces used by Jia and Liu (*Adv. Comput. Math..*, 77 (2007), 287–312) in their construction of wavelet bases which generate Riesz bases for $H^s(\Omega)$, with $s \in (1.618, \frac{5}{2})$. The idea of such bases is to construct them recursively by adding to the basis from the previous approximation space a set of locally supported functions spanning a complement space such that the union is a basis of the current approximation space. In particular, we will use hierarchical bases meaning that the functions that are added are just a subset of a basis for the space on the current level. The starting point for our construction is the Lagrange basis constructed by Nürnberger and Zeilfelder (*Proceedings Multivariate Approximation*. Birhäuser, Basel, 2001) for C^1 piecewise quadratic polynomials on Powell-Sabin-6 triangulations of arbitrary polygonal domains. With slight modification to the construction of NZ01 on the initial level and another algorithm developed for successive refinement levels we construct nested Lagrange interpolation sets, which is the key step in the construction of hierarchical bases. Compared to the Riesz bases con-

structed by Jia and Liu, our Riesz bases have a bigger range of stability, and to the earlier hierarchical Riesz bases for $H^s(\Omega)$, $s \in (1, \frac{5}{2})$ of also Lagrange type constructed by Davydov and Stevenson on checkerboard quadrangulations, our construction is an advantage over (O. Davydov and R. Stevenson, Hierarchical Riesz bases for $H^s(\Omega)$, $1 < s < \frac{5}{2}$, *Constr. Approx.*, 22 (2005), 365–394), as it applies to general triangulations of arbitrary polygonal domains. Since the range of stability of our Riesz bases for $H^s(\Omega)$ also includes $s = 2$ like the other two constructions, we plan to explore the use of the corresponding hierarchical basis in preconditioning the fourth order elliptic problems such that the stiffness matrices will be uniformly well-conditioned.

The numerical linear algebra of approximation involving Radial Basis Functions

Shengxin Zhu & Andy Wathen *(University of Oxford)*

Radial Basis Functions have attracted a lot of attentions in recent years as an elegant approximation scheme for multidimensional data and an attractive way to solve partial differential equations. These methods share many advantages, being meshfree/meshless in any dimension, and having good approximation properties, however they lead to significant problems of linear algebra—the related linear systems of equations are always highly ill-conditioned. Thus constructing effective fast solvers plays an important role in practical use of these methods and will shape their future utility for large scale problems. We are going talk about issues related to coping with the severely ill-conditoned systems as well as bringing some open problems.

Tuesday 28th June

Chair:	K3.25: Ainsworth		
9:00-9:05	Opening Remarks		
9:05-10:05	**R Schaback** Kernel-Based Meshless Methods for Solving PDEs		
10:05-11:05	**R Skeel** The best of fast N-body methods		
11:05–11:30	COFFEE/TEA		
Chair:	K3.25: M1	K3.14: M2	K3.17: M4
11:30-11:55	**S Repin** M1 A posteriori estimates for problems with linear growth energy functionals	**L N Trefethen** M2 Convergence theorems for polynomial interpolation in Chebyshev points	**P Burrage** M4 Using a modification of the SSA to simulate spatial aspects of chemical kinetics
11:55-12:20	**S Micheletti** M1 Anisotropic mesh adaptation via a posteriori error estimation	**M Richardson** M2 Approximating functions with endpoint Singularities	**A Lang** M4 Lax's equivalence theorem for stochastic differential equations
12:20-12:45	**A Allendes** M1 A posteriori error estimation and an adaptive scheme for the choice of the stabilization parameter in low-order finite element approximations of the Stokes problem	**R Pachón** M2 Getting rid of spurious poles: a practical approach	**K Burrage** M4 From cells to tissue: coping with heterogeneity via fractional models
12:45-14:00	LUNCH-Lord Todd		
Chair:	K3.25: Knight		
14:00-15:00	**L N Trefethen** Six myths of polynomial interpolation and quadrature		
Chair:	K3.25: M1	K3.14: M3	K3.17: M4
15:00-15:25	**M Maischak** M1 Error estimators for a partially clamped plate problem with bem	**A Birkisson** M3 Automatic differentiation for automatic solution of nonlinear BVPs	**M Riedler** M4 Numerical Simulation of Stochastic Reaction Networks modelled by Piecewise Deterministic Markov Processes
15:25-15:50	**O Lakkis** M1 A finite element method for nonlinear elliptic equations	**N Hale** M3 "Rectangular pseudospectral differentiation matrices" or, "Why it's not hip to be square"	**A Barth** M4 Multilevel Monte Carlo Finite Element Methods for Elliptic PDEs with Stochastic Coefficients
15:50-16:15	**N Kopteva** M1 A posteriori error estimates for classical and singularly perturbed parabolic equations	**P Gonnet** M3 Finite difference preconditioners for spectral methods	**L Szpruch** M4 Efficient Multilevel Monte Carlo simulations of non-linear financial SDEs without a need of simulating Levy areas
16:15-16:45	COFFEE/TEA		
Chair:	K3.25: Watson		
16:45-17:55	**A Quarteroni (A.R. Mitchell Lecture)** Mathematical models for the cardiovascular system: analysis, numerical simulation, applications		
18:15-19:15	DINNER-Lord Todd		
20:00-22:00	RECEPTION-Glasgow City Chambers		

M1 A-posteriori error estimation, M2 Approximation with polynomials, M3 Novel algorithms for BVPs, M4 Stochastic computation

11:05–11:30	COFFEE/TEA	
Chair:	K4.12: M5	K3.27: Abelman
11:30-11:55	**S Loisel** M5 Sharp performance estimates for optimized domain decomposition preconditioners	**E Sousa** A Lax-Wendroff type numerical method for a fractional advection diffusion equation
11:55-12:20	**K Chen** M5 Fast Multigrid Algorithms and High Order Variational Image Registration Model	**R Brown** Using reduced-order models and waveform relaxation to solve cerebral bloodflow autoregulation DEs on a large binary tree network
12:20-12:45	**D Loghin** M5 Interface preconditioners for flow problems	**C Brezinski** Nonlinear functional equations satisfied by orthogonal polynomials
12:45-14:00	LUNCH-Lord Todd	
Chair:	K4.12: M5	K3.27: Davis
15:00-15:25	**D Silvester** M5 Fast Iterative Solvers for Saddle Point Problems	**M Redivo-Zaglia** Hirota's bilinear method and the ε–algorithm
15:25-15:50	**A Ramage** M5 Saddle-point Problems in Liquid Crystal Modelling	**F Schieweck** Higher order variational time discretizations for nonlinear systems of ordinary differential equations
15:50-16:15	**J Pearson** M5 Preconditioned Iterative Methods for Convection-Diffusion Control Problems	**S Güttel** A parallel integrator for linear initial-value problems
16:15-16:45	COFFEE/TEA	

Wednesday 29th June

Chair:	K3.25: Higham		
9:00-10:00	**B Wohlmuth** Finite element approximations for coupled problems		
10:00-11:00	**J Nocedal** Optimization Methods for Machine Learning		
11:00–11:30	COFFEE/TEA		
Chair:	K3.25: M1	K3.14: M4	K3.17: M6
11:30-11:55	**V M Vohralik** M1 A unified framework for a posteriori error estimation for the Stokes problem	**M Roj** M4 Mean Exit Times and Multi-Level Monte Carlo Simulations	**S Kirkland** M6 Bipartite Subgraphs and the Signless Laplacian Matrix
11:55-12:20	**R Rankin** M1 A posteriori error estimation for finite element approximations of linear elasticity problems	**R Kruse** M4 Optimal Error Estimates of Galerkin Finite Element Methods for SPDEs with Multiplicative Noise	**M Musolesi** M6 Temporal Graphs and Robustness
12:20-12:45	**E Verhille** M1 A posteriori error estimator for the Reissner-Mindlin problem	**E Buckwar** M4 Linear Stability Analysis of Numerical Methods for Stochastic Differential Equations	**M McDonald** M6 Networks in Neuroscience: Using the Generalised Singular Value Decomposition to Compare Pairs of Networks
12:45-14:00	LUNCH-Lord Todd		
Chair:	K3.25: Mackenzie		
14:00-15:00	**C Johnson** Image-Based Biomedical Modeling, Simulation and Visualization		
Chair:	K3.25: M1	K3.14: M4	K3.17: M6
15:00-15:25	**E Georgoulis** M1 A posteriori error estimates for linear wave problems	**W Liu** M4 Euler–Maruyama-type Numerical Methods for Stochastic Lotka-Volterra Model	**C Lee** M6 Reordering multiple networks
15:25-15:50	**S Nicaise** M1 A residual-based a posteriori estimator for the $\mathbf{A} - \varphi$ magneto-dynamic harmonic formulation of the Maxwell system	**G dos Reis** M4 Numerics for Quadratic FBSDE	**J Crofts** M6 Googling the brain: Discovering hierarchical and asymmetric structure, with applications to neuroscience
15:50-16:15	**L Asner** *A posteriori* error estimation for coupled problems	**P Taylor** M4 Adaptive stepsize control for the strong numerical solution of SDEs	**D Higham** M6 Bistability Through Triad Closure
16:15-16:45	COFFEE/TEA		
Chair:	K3.25: Brunner	K3.14: Langdon	K3.17: M6
16:45-17:10	**P J Davies** Convolution quadrature revisited for Volterra integral equations	**A Teckentrup** Multilevel Monte Carlo for highly heterogeneous media	**A Mantzaris** M6 Dynamic Communicators
17:10-17:35	**T Okayama** Theoretical analysis of Sinc-collocation methods for weakly singular Volterra integral equations of the second kind	**T Moroney** An efficient finite volume method applied to flow in heterogeneous porous media	**C Phokaew** M6 A graph model to explain the origin of early proteins
17:35-18:00	**R Fernandes** Comparing two iterated projection approximations for integral operators in terms of convergence and computational cost	**D Duncan** Postprocessing Reservoir Simulations to Obtain Accurate Well Pressures	**Z Stoyanov** M6 Communicability of networks
18:30-19:30	DINNER-Lord Todd		

M1 A-posteriori error estimation, M4 Stochastic computation, M6 Complex Networks and Matrix Computations

Wednesday 29th June

11:00–11:30	COFFEE/TEA	
Chair:	K4.12: Garcia-Archilla	K3.27: Hall
11:30-11:55	**JP Berrut** A formula for the influence of jumps on finite sinc interpolants	**M J D Powell** The augmented Lagrangian method with bounds on the dual variables
11:55-12:20	**G Klein** Linear rational finite differences and applications	**R Fletcher** Limited memory spectral gradient methods
12:20-12:45	**A F Rabarison** Algorithm and error bounds for piecewise linear approximation on anisotropic triangulations	**N Gould** Puiseux-based extrapolation for large-scale degenerate quadratic programming
12:45-14:00	LUNCH-Lord Todd	

Chair:	K4.12: Stynes	K3.27: Fletcher
15:00-15:25	**A Townsend** Multiscale analysis in Sobolev Spaces on bounded domains with restricted interpolation points	**Q Huangfu** A high performance dual simplex solver
15:25-15:50	**O Davydov** RBF-FD Methods for Elliptic Equations	**J Hall** Matrix-free IPM with GPU acceleration
15:50-16:15	**G Andriamaro** Bernstein-Bézier Finite Elements	**J Hogg** Experience of linear solvers in an nonlinear interior point method
16:15-16:45	COFFEE/TEA	
Chair:	K4.12: Scheichl	K3.27: Ergül
16:45-17:10	**O Türk** Chebyshev spectral collocation method for unsteady MHD flow and heat transfer between parallel plates	**N K Nichols** Optimal state and parameter estimation using a hybrid data assimilation scheme
17:10-17:35	**C Varsakelis** Numerical analysis of two-phase granular flows at low Mach numbers	**S Jenkins** The Effects of Dispersive and Dissipative Properties of Numerical Methods on the Linear Advection Equation during Data Assimilation
17:35-18:00	**S Abelman** Reduction and solutions for unsteady flow of a Sisko fluid for cylindrical geometry	**D Partridge** Using data assimilation within a moving mesh approach to ice sheet modelling
18:30-19:30	DINNER-Lord Todd	

Thursday 30th June

Chair:	K3.25: Barrenechea		
9:00-10:00	**O Bruno** Spectral frequency- and time-domain PDE solvers for general domains		
10:00-11:00	**R Tempone** Error estimates and adaptive algorithms for single and multievel Monte Carlo Simulation of Stochastic Differential Equations		
11:00–11:30	COFFEE/TEA		
Chair:	K3.25: M7	K3.14: M8	K3.17: M9
11:30-11:55	**B Garcia-Archilla** M7 Stabilization of convection-diffusion problems by Shishkin mesh simulation	**R Borsdorf** M8 Two Two-Sided Procrustes Problems Arising in Atomic Chemistry	**M Ainsworth** M9 Optimally blended finite element-spectral element schemes for wave propagation
11:55-12:20	**J L Gracia** M7 Time and space-accurate numerical solution of one-dimensional parabolic singularly perturbed problems of reaction-diffusion type	**E Deadman** M8 Blocked Methods for Computing the Square Root of a Matrix	**T Betcke** M9 Recent Developments in nonpolynomial finite element methods for wave problems
12:20-12:45	**T Linß** M7 Collocation methods for singularly perturbed reaction-diffusion equations	**P Knight** M8 A Linear Algebraist's Approach to Reforming The UK Voting System	**Ö Ergül** M9 Extremely Large Electromagnetics Problems: Are We Going in the Right Direction ?
12:45-14:00	LUNCH-Lord Todd		
Chair:	K3.25: Ramage		
14:00-15:00	**J Dongarra** On the Future of High Performance Computing: How to Think for Peta and Exascale Computing		
Chair:	K3.25: M7	K3.14: M8	K3.17: M9
15:00-15:25	**L Ludwig** M7 Supercloseness of the SDFEM for convection-diffusion problems with reduced regularity	**A Spence** M8 A method for the computation of Jordan blocks in parameter-dependent matrices	**S Langdon** M9 A high frequency boundary element method for scattering by non-convex obstacles
15:25-15:50	**J Quinn** M7 A Linear Singularly Perturbed Problem with an Interior Turning Point	**A Wathen** M8 Preconditioning for GMRES	**L Gao** Energy Conservation Laws of Maxwell's Equations and Their Application in Numerical Analysis of FDTD
15:50-16:15	**M Stynes** M7 A balanced finite element method for singularly perturbed reaction-diffusion problems	**F Tisseur** Structure Preserving Transformations for Quadratic Matrix Polynomials	**A Bespalov** Differential complexes and interpolation operators in the context of high-order numerical methods for electromagnetic problems
16:15-16:45	COFFEE/TEA		
Chair:	K3.25: Linß	K3.14: Deadman	K3.17: Duncan
16:45-17:10	**J Mackenzie** Robust Solution of a BVP arising in Liquid Crystal Modelling	**L Lin** Fractional Matrix Powers	**B Pekmen** DQM Time-DQM Space Solution of Hyperbolic Telegraph Equation
17:10-17:35	**J Van lent** Distributing Points in a Triangle using Optimal Transport Techniques	**S Miyajima** The relation between two algorithms for enclosing matrix eigenvalues	**N Akgün** DRBEM and DQM Solutions of Natural Convection Flow in a Cavity Under a Magnetic Field
17:35-18:00	**A Araújo** Stability and convergence of finite difference schemes for complex diffusion processes	**Y Nakatsukasa** Arithmetic and communication minimizing algorithms for the symmetric eigendecomposition and the singular value decomposition	**M Tezer-Sezgin** MHD flow and heat transfer between parallel plates with Navier-slip wall condition
19:00 for 19:30	DRINKS RECEPTION and CONFERENCE DINNER-Lord Todd		

M7 Singularly perturbed problems, M8 Numerical Linear Algebra, M9 High frequency and oscillatory problems

11:00–11:30		COFFEE/TEA	
Chair:	K4.12: Silvester	K3.27: Berrut	AR201: K Burrage
11:30-11:55	**M Payne** Dual Lumping of Isogeometric Finite Element Schemes using Petrov-Galerkin Techniques	**C Brito-Loeza** On numerical algorithms for level set and curvature based models for surface fairing	**Q Yang** Novel numerical methods for nonlinear time-space fractional diffusion equations in two dimensions
11:55-12:20	**R Scheichl** Energy Minimizing Coarse Spaces with Functional Constraints	**L Sun** A new splitting method for mean curvature-based variational image denoising	**A Khan** Convergence of an implicit algorithm for a finite family of asymptotically quasi-nonexpansive maps
12:20-12:45	**J Phillips** Finite elements on pyramids	**W Yeo** C^1 Piecewise Quadratic Hierarchical Bases	**D Altintan** How to solve boundary value problems by using Variational Iteration Method
12:45-14:00		LUNCH-Lord Todd	

Chair:	K4.12: Georgoulis	K3.27: Loisel	AR201: Nichols
15:00-15:25	**G Barrenechea** A low order local projection stabilized finite element method for the Oseen equation	**D Janovská** Zeros of matrix polynomials: A case study	**U Ruede** Towards Exascale Computing: Multilevel Methods and Flow Solvers for Millions of Cores
15:25-15:50	**A Cangiani** Mimetic Finite Difference methods for elliptic problems	**R Kammogne** Domain Decomposition for Reaction-Diffusion Systems	**J Lanzoni** Norm growth and pseudospectra for PML discretisations of open systems
15:50-16:15	**A Saeed** Numerical Solution of Fully Nonlinear Elliptic PDEs with a Modified Argyris Element	**PG Martinsson** Fast Direct Solvers for Elliptic PDEs	**D Tang** iGen: a program for the automated generation of reduced-dimension models
16:15-16:45		COFFEE/TEA	
Chair:	K4.12: Cangiani	K3.27: Gould	
16:45-17:10	**T Kang** $T-\psi$ finite element schemes for eddy current problems	**S Zhu** The numerical linear algebra of approximation involving Radial Basis Functions	
17:10-17:35	**T Horváth** A fast matrix assembley for interior penalty discontinuous Galerkin method	**H Wang** A Posteriori Error Analysis for a Quasicontinuum Method	
17:35-18:00	**V Janovsky** On periodic patterns in the traffic flow	**M Al-Baali** Convergence analysis of a family of damped quasi-Newton methods for nonlinear optimization	
19:00 for 19:30		DRINKS RECEPTION and CONFERENCE DINNER-Lord Todd	

Friday 1st July

Chair:	K3.25: Davydov		
9:00-10:00	**D Perić** On Computational Strategies for Fluid-Structure Interaction: Some Insights into Algorithmic Basis with Applications		
10:00-11:00	**J Nagy** Numerical Methods for Large Scale Inverse Problems in Image Reconstruction		
11:00–11:30	COFFEE/TEA		
Chair:	K3.25: M10	K3.14: M11	K3.27: M12
11:30-11:55	**E Tyrtyshnikov** M10 Matrix computations with data in multi-index formats	**O Devolder** M11 The Fast Gradient Method as a Universal Optimal First-Order Method	**J Blanchard** M12 GPU Accelerated Greedy Algorithms for Sparse Approximation
11:55-12:20	**D Savostyanov** M10 Rank-one QTT vectors with QTT rank-one and full-rank Fourier images	**M Takac** M11 Efficiency of Randomized Coordinate Descent Methods on Minimization Problems with a Composite Objective Function	**P Richtarik** M12 A GPU accelerated coordinate descent method for large-scale L1-regularised convex minimization
12:20-12:45	**P Zhlobich** M10 Stability of QR-based system solvers for a subclass of Quasiseperable Order One matrices	**M Kocvara** M11 Solving topology optimization problems by domain decomposition	**M Lotz** M12 Compressed sensing thresholds and condition numbers in optimization
12:45-13:10			**A Thompson** M12 A new recovery analysis of Iterative Hard Thresholding for Compressed Sensing
13:15-14:30	LUNCH-Foyer outside K3.25		
	END OF CONFERENCE		

M10 Linear algebra in data-sparse representations, M11 Optimization: complexity and applications, M12 Compressed Sensing: algorithms and theory