25th Biennial Conference on Numerical Analysis

25 June - 28 June, 2013

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Introduction

Dear Participant,

On behalf of the Strathclyde Numerical Analysis and Scientific Computing Group, it is our pleasure to welcome you to the 25th Biennial Numerical Analysis conference. This is the third time the meeting has been held at Strathclyde, continuing the long series of conferences originally hosted in Dundee.

The conference is rather unusual in the sense that it seeks to encompass all areas of numerical analysis, and the list of invited speakers reflects this aim. We have once again been extremely fortunate in securing, what we hope you will agree is, an impressive line up of eminent plenary speakers.

The meeting is funded almost entirely from the registration fees of the participants. However, 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 and supporting the attendance of several UK-based PhD students. Additional financial support for some overseas participants has come from the *Dundee Numerical Analysis Fund*, started by Professor Gene Golub from Stanford University in 2007. Finally, 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 2015 to celebrate 50 years of Biennial Numerical Analysis conferences in Scotland!

Philip Knight
John Mackenzie
Alison Ramage

Conference Organising Committee

Information for participants

- **General**. There will be a registration desk in the foyer of the John Anderson building (building 16 on the campus map, entry on Level 4 from Taylor Street as indicated). The conference office will be located in the Cluster Manager's office, room JA412a 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 JA326.
- **Meals**. Most meals 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. Lunch on Thursday will be in the Java Cafe in the Sir William Duncan building (no. 18 on the map). A buffet lunch will be served on Friday in the foyer outside JA325.
- **Lecture rooms**. These are mainly in the John Anderson building (building 16, enter on Level 4 from Taylor Street). The main auditorium (JA325) is down one floor from the main entrance, along with rooms JA314, JA317, JA326 and JA327. The additional rooms for parallel sessions are JA412 (on the entrance level of the John Anderson building near the registration desk), JA505 and JA507 (on level 5 in John Anderson) 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 JA325.
- **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 25th June from 20.00 to 21.00. The City Chambers is marked on the campus map: entry is from George Square.
- **Conference dinner**. The conference dinner will be held in the Lord Todd Dining Room on Thursday 27th June at 19.00 for 19:30. The guest speaker will be Professor Des Higham, University of Strathclyde.
- **Book displays**. There will be books on display for the duration of the conference in room JA326.
- **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 CV309 of the Colville Building. This room can be accessed from the John Anderson building (past lecture rooms JA314 and JA317) 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.

Invited Speakers

Assyr Abdulle	EPF de Lausanne	assyr.abdulle@epfl.ch
Rick Beatson	University of Canterbury	rick.beatson@canterbury.ac.nz
Pavel Bochev	Sandia National Labs	pbboche@sandia.gov
Hermann Brunner	Memorial University	hbrunner@math.hkbu.edu.hk
Monique Dauge	University of Rennes	monique.dauge@univ-rennes1.fr
Juan Meza	University of California	jcmeza@ucmerced.edu
Peter Monk	University of Delaware	monk@math.udel.edu
Dianne O'Leary	University of Maryland	oleary@cs.umd.edu
Mike Powell	University of Cambridge	mjdp@damtp.cam.ac.uk
Ian Sloan	University of New South Wales	i.sloan@unsw.edu.au
Tao Tang	Hong Kong Baptist University	ttang@hkbu.edu.hk
Jared Tanner	University of Oxford	tanner@maths.ox.ac.uk

Abstracts of Invited Talks

Numerical homogenization methods: beyond a story of sand

Assyr Abdulle *(EPF de Lausanne)*

Starting with the famous constitutive law for the flow of a fluid through a column of sand proposed by Henry Darcy in the mid 18th century, we will discuss the various scales hidden in such a physical process and briefly introduce the notion of homogenization.

We will then present recent developments in the design and analysis of numerical homogenization methods. In particular, we will discuss reduced order modeling for the numerical homogenization of nonlinear problems and adaptive multiscale methods that couple Stokes and Darcy problems.

Radial basis functions applications and theory

Rick Beatson *(University of Canterbury)*

In common with many fields within numerical analysis and approximation theory, radial basis functions is a continuum of questions (and answers) of different types. These may be function theoretic, algorithmic, computational, or may be directly connected with a particular application.

In this talk I will start at the applied end with a selection of applications of radial basis functions. The emphasis will be on several applications connected with applied geology. Radial basis functions have been very successful in these applications where the data is typically scattered and sparse.

The latter part of the talk will concern work of a more function theoretic nature. I will discuss sufficient conditions for a zonal kernel to be strictly positive definite on the sphere $\mathbb{S}^{d-1}$. Such kernels lead to interpolation systems which ae uniquely solvable, no matter the position of the nodes. The sufficient conditions for positive definiteness, developed in collaboration with Wolfgang zu Castell and Yuan Xu, lead to families of compactly supported strictly positive definite zonal kernels on spheres. There are also dimension hopping operators which generate smoother positive definite kernels on $\mathbb{S}^{d-1}$ from those on $\mathbb{S}^{d+1}$, or less smooth positive definite kernels on $\mathbb{S}^{d+1}$ from those for $\mathbb{S}^{d-1}$. The end result is many new members for the zoo of compactly supported zonal kernels.

Optimization-based modeling - a new strategy for predictive simulations of multiscale, multiphysics problems

Pavel Bochev (*Sandia National Laboratories*)

Optimization-based modeling (OBM) is a "divide-and-conquer" strategy that decomposes mutiphysics, multiscale operators into simpler constituent components and separates preservation of physical properties such as a discrete maximum principle, local bounds, or monotonicity from the discretization process. In so doing OBM relieves discretization from tasks that impose severe geometric constraints on the mesh, or tangle accuracy and resolution with the preservation of physical properties.

In a nutshell, our approach reformulates a given mathematical model into an equivalent *multi-objective constrained optimization problem.* The optimization objective is to minimize the discrepancy between a *target* approximate solution and a *state*, subject to constraints derived from the component physics operators and the condition that physical properties are preserved in the optimal solution. Three examples will illustrate the scope of our approach: (1) an optimization-based framework for the synthesis of robust, scalable solvers for multiphysics problems from fast solvers for their constituent physics components; (2) an optimization-based Atomistic-to-Continuum (AtC) coupling method; and (3) optimization-based methods for constrained interpolation (remap) and conservative, monotone transport.

This talk is based on joint work with Denis Ridzal, Kara Peterson, Mitch Luskin, Derek Olson, Alex Shapeev, and Misha Shashkov. This research is supported by the Applied Mathematics Program within the Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR). The work on AtC coupling methods is supported by the ASCR as part of the Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4).

Numerical analysis and computational solution of integro-differential equations

Hermann Brunner (*Memorial University of Newfoundland* and *Hong Kong Baptist University*)

Volterra first studied (partial) integro-differential equations in his papers of 1909 and 1912, and he observed in the latter that in order to solve such problems "it is necessary to employ an analysis that is rather different from the one used for differential or integral equations". This observation applies equally to the numerical analysis and the computational solution of

ordinary and partial Volterra integro-differential equations (VIDEs), not least because in the mathematical modelling of hereditary phenomena these equations often occur in non-standard forms. I will describe typical examples of such integro-differential equations in the first part of my talk. This will be followed by a brief review of theoretical aspects of important classes of time-stepping schemes (collocation methods; discontinuous Galerkin methods and their *hp*-versions; methods based on convolution quadrature) for ordinary and partial VIDEs. In the last part of the talk I shall describe some recent approaches to the computational solution of non-standard VIDEs and show that many challenging problems remain to be addressed.

Old and New on eigenvalues of the Schur complement of the Stokes operator

Monique Dauge & Martin Costabel *(University of Rennes)*

The lowest eigenvalue of the Schur complement of the Stokes operator coincides with the square of the inf-sup constant of the divergence, also called LBB constant (after Ladyzhenskaya, Babuska and Brezzi). This quantity receives much attention in the literature. Most of available results are for two dimensional domains. In a widely know paper [1], Horgan & Payne relate this constant with the Friedrichs constant and deduce a simple lower bound for the LBB constant. This lower bound was popularized as the Horgan & Payne angle.

We discovered recently that the proof of H&P is flawed. Later on we found a counter-example founded on theoretical and computational arguments. In this talk I will tell this story, and also some positive results we were able to prove, improving a recent result by Duran [2] for two-dimensional domains.

This talk is partly based on the preprint [3], and ongoing collaboration with Michel Crouzeix and Yvon Lafranche (Univ. Rennes 1), Christine Bernardi and Vivette Girault (Univ. P&M Curie).

[1] C.O. Horgan, L.E. Payne – On inequalities of Korn, Friedrichs and Babuska–Aziz, Arch. Rat. Mech. Anal., 82 (1983), 165–179.
[2] R.G. Duran – An elementary proof of the continuity from $L2_0(\Omega)$ to $H1_0(\Omega)^n$ of Bogovskii's right inverse of the divergence. Revista de la Unión Matemática Argentina, 53 (2012), 59–78.
[3] M. Costabel, M. Dauge – On the inequalities of Babuska-Aziz, Friedrichs and Horgan-Payne, Prepublication Rennes, Mars 2013. http://fr.arxiv.org/abs/1303.6141

Mathematical Challenges and Opportunities in Energy and the Environment

Juan C. Meza *(University of California, Merced)*

The current emphasis on reducing our carbon footprint to minimize the impact on climate change has resulted in a renewed interest in energy and the environment. Both of these fields present numerous opportunities for numerical analysts to work in. With the advance of new mathematical algorithms and high performance computers, we can now study techniques for reducing our carbon footprint such as carbon capture and sequestration and new renewable energy sources. This talk will present an overview of some of the challenges in the development of alternative energy sources and their effect on existing systems such as the electric power grid. These challenges provide an excellent source of new applications for numerical analysts. I will discuss one area in detail, the computation of the electronic structure of materials. The electronic structure problem is a long-standing problem that can be used to predict and design materials for many applications, such as new and more efficient solar cells. I will present an approach based on an optimization method that directly minimizes the Kohn-Sham total energy. Numerical experiments demonstrate that the combination of this new optimization method is more efficient and robust than previous methods.

The solution of time harmonic wave equations using complete families of elementary solutions

Peter Monk *(University of Delaware)*

I shall discuss plane wave methods for approximating time-harmonic wave equations paying particular attention to the Ultra Weak Variational Formulation (UWVF). This method is essentially a Discontinuous Galerkin method in which the approximating basis functions are special traces of solutions of the underlying wave equation. In the classical UWVF due to Cessenat and Després, sums of plane wave solutions are used element by element to approximate the global solution. For these basis functions, convergence analysis and considerable computational experience shows that, under mesh refinement, the method exhibits a high order of convergence depending on the number of plane wave used on each element.

I will present recent applications of the UWVF to the elastic wave equation and to a biharmonic problem. The latter problem requires the use of both traveling wave solutions and exponentially varying solutions.

Of course plane wave methods are limited to approx-

imating problems with piecewise constant (or slowly varying) parameters. In some applications this is not realistic and so it is necessary to extend the method to the case of smoothly varying parameters. I shall comment on attempts to mitigate this problem also.

Image Restoration and Uncertainty Quantification

Dianne P. O'Leary *(University of Maryland)*

High quality images are essential in scientific discovery, forensics, and medical diagnosis. Images can be degraded by blur caused by lens or atmospheric effects, by motion of the subject, or by defective recording devices.

The talk will focus on using ideas from machine learning and scientific computing to guide us to improved estimates of the true image and of the uncertainty in our estimate. The methods include providing evaluation tools, exploiting training data, using Bayesian estimation, and designing optimal filters.

Some of this work is joint with Julianne Chung, Matthias Chung, Brianna Cash, and Viktoria Taroudaki.

On the symmetric Broyden formula in optimization calculations

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

Let the least value of a function $F(x)$, $x \in \mathcal{R}^n$, be required when second derivatives are not available. It is helpful to construct and to update a quadratic approximation Q to F, so that changes to the variables can be guided by reductions in Q. The symmetric Broyden method is a highly successful technique for updating $\nabla^2 Q$ using only of magnitude n data, for example one change in gradient $\nabla F(x+d)-\nabla F(x)$, which occurs if the step d is taken from x in the space of the variables. The new model Q interpolates these data, and the freedom is taken up by minimizing the Frobenius norm of the change to the second derivative matrix of the model.

It follows that, if F happens to be quadratic, then every update that alters $\nabla^2 Q$ provides a reduction in the error $\|\nabla^2 Q-\nabla^2 F\|_F$, where the subscript F denotes the Frobenius matrix norm. Furthermore, sequences of updates give changes to $\nabla^2 Q$ that tend to zero. We investigate these fundamental properties by numerical experiments when F is a strictly convex quadratic function whose first derivatives are available. The changes to x are generated by a trust region method, which means that each new vector of variables is an estimate of the vector that minimizes Q within a certain distance of the best vector so far. We give particular attention to the magnitudes of the final values of $\|\nabla^2 Q-\nabla^2 F\|_F$.

The symmetric Broyden formula is useful too without any derivatives of F. Then second derivative information is supplied in the updating of Q by interpolation to values of F at more than $n+1$ points, a typical number of points being $2n+1$. Their positions have to be maintained so that interpolation by a quadratic is possible for any right hand sides. This is done in the NEWUOA software of the author, for example. We compare some numerical results of this software with the experiments mentioned in the previous paragraph. Also an extension of NEWUOA that allows general linear constraints on the variables is addressed briefly. A feature of all of this software, which allows it to be applied when there are hundreds of variables and no sparsity, is that the average amount of routine work of each iteration is only of magnitude n^2.

Lifting the Curse of Dimensionality: Numerical Integration in Very High Dimensions

Ian H. Sloan *(University of New South Wales)*

Richard Bellman coined the phrase "the curse of dimensionality" to describe the extraordinarily rapid increase in the difficulty of most problems as the number of variables increases. One such problem is numerical multiple integration, where the cost of any integration formula of product type obviously rises exponentially with the number of variables. Nevertheless, problems with hundreds or even thousands of variables do arise, and are now being tackled successfully. In this talk I will tell the story of recent developments, in which within a decade the focus turned from existence theorems to concrete constructions that achieve the theoretically predicted results even for integrals in hundreds or thousands of dimensions and many thousands of points. The theory has been shaped by applications, ranging from option pricing to the flow of a liquid through a porous medium, the latter modelled by a partial differential equation with a random permeability field.

High-Order and Adaptive Time Stepping Methods for Energy Gradient Flows

Tao Tang *(Hong Kong Baptist University)*

The phase-field method is very useful for modeling interfacial phenomena. The key idea of the phase-field methodology is to replace sharp interfaces by thin transition regions where interfacial forces are smoothly distributed. One of the main reasons for the success of the phase-field methodology is that it is based

on rigorous mathematics and thermodynamics. Most phase-field models satisfy a nonlinear stability relationship, usually expressed as a time-decreasing free-energy functional, which is called energy gradient stability. To obtain accurate numerical solutions of such problems, it is desirable to use high-order approximations in space and time. Yet because of the difficulties introduced by the combination of nonlinearity and stiffness, most computations have been limited to lower-order in time, and in most cases to constant time-stepping. On the other hand, numerical simulations for many physical problems require large time integration; as a result large time-stepping methods become necessary in some time regimes. To effectively solve the relevant physical problems, the combination of higher-order and highly stable temporal discretizations becomes very useful. In this talk, we will describe some adaptive time stepping approach for phase-field problems, which inherits the energy gradient stability of the continuous model. Particular attention will be given to effectively resolve both the solution dynamics and steady state solutions.

Sparse compressed sensing and matrix completion

Jared Tanner, Bubacarr Bah & Ke Wei *(University of Oxford)*

The essential information in large data sets is typically contained in a low dimensional subspace of the space in which the data is observed or collected. For instance, natural images are highly compressible in standard wavelet bases and many matrices are well approximated by a low rank approximation. Prior knowledge that the data has an underlying simplicity allows data to be acquired at a rate proportional to the information content as opposed to the ambient space in which the data is represented. Namely, signals/images which are known to be compressible in a given basis can be fully recovered from their inner product with few random vectors, and matrices which are low rank can be determined from a subset of their entries. We discuss recent advances in these topics of compressed sensing and matrix completion, focusing on maximally sparse sampling operators and recovery using algorithms that directly solve the natural non-convex formulation of these questions. In particular, we present provable bounds for expander graphs suitable for compressed sensing measurements and show preliminary evidence that simple alternating projection algorithms can efficiently recover low rank matrices with the number of measurements approaching their respective degrees of freedom.

Minisymposia abstracts

Minisymposium M1

Recent Advances in Big Data Problems
Organisers
Martin Takáč and Rachael Tappenden

Doubly Parallelized Coordinate Descent

Olivier Fercoq & Peter Richtárik *(University of Edinburgh)*

We study the combination of two ways of parallelizing the randomized coordinate descent method. The first one is the Parallel Coordinate Descent Method [1] where several coordinate descent iterates are performed in parallel in order to get a larger objective decrease at each iteration. The second one is Monte Carlo parallelization, successfully applied to stochastic gradient in [2], where we perform several times in parallel the same randomized algorithm in order to reduce the probability that the sequence of random iterates results in finding the solution in many more iterations than what is most of the time observed. Combining the two parallelizations gives the Doubly Parallelized Coordinate Descent Method.

Let $\tilde{K}(\tau, q)$ denote the iteration complexity of a parallel randomized optimization algorithm to obtain an ϵ-solution with probability at least $1-q$ when using τ processors and suppose we have T processors. The question we are studying in this paper is to search for the fastest of all the allocations of these T processors to obtain an ϵ-solution with probability at least $1-\rho$ with $\rho \leq q$. This can be formulated as an optimization problem on the set of divisors of T:

$$\min_{r|T} \tilde{K}(T/r, \rho^{1/r}) \ .$$

We show that there exists an allocation of processors among the two levels of parallelism, that gives the smallest theoretical complexity for the Doubly Parallelized Coordinate Descent Method. Depending on the problem at stake, both approaches may be competitive, or a nested parallelism may be better.

Then we present an experimental insight on the allocation of processors among both levels of parallelism. We show that the actual behaviour of the algorithm is of course related to its theoretical complexity but that the optimal allocation of processors for fastest actual decrease can be different than the optimal allocation for smallest theoretical iteration complexity.

Finally, we present a simple model of communication delays within a cluster of computers that shows that the longer communication delays, the more Monte Carlo parallelism should be considered.

[1] Peter Richtarik and Martin Takac. Parallel coordinate descent methods for big data optimization problems. arXiv:1212.0873, November 2012.
[2] Martin Zinkevich, Markus Weimer, Alex Smola, and Lihong Li. Parallelized stochastic gradient descent. Advances in Neural Information Processing Systems, 23(23):19, 2010.

Randomized lock-free methods for minimizing partially separable convex functions

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

We develop and study the iteration complexity of a class of randomized parallel lock-free (asynchronous) first-order methods applied to the problem of minimizing a partially separable convex function. Our methods are especially well suited for big data optimization applications.

In special cases our generic algorithm reduces to parallel gradient descent, parallel stochastic gradient descent, parallel randomized block coordinate descent and Hogwild! [1]. In all cases our results are the first complexity estimates for lock-free variants of the methods, with the exception of Hogwild!, which was analyzed before, and for which we give vastly improved complexity results.

We contrast the approach with the efficiency of synchronous parallel coordinate descent methods [2] applied to the same problem.

[1] F. Niu, B. Recht, C. Re, and S. Wright, Hogwild!: A lock-free approach to parallelizing stochastic gradient descent, NIPS 2011.
[2] P. Richtárik and M. Takáč, Parallel coordinate descent methods for big data optimization, arXiv:1212:0873, 2012.

Alternating maximization: unifying framework for 8 sparse PCA formulations and efficient parallel codes

Martin Takáč & Peter Richtárik & Selin Damla Ahipaşaoğlu *(University of Edinburgh)*

Given a multivariate data set, sparse principal component analysis (SPCA) aims to extract several linear combinations of the variables that together explain the variance in the data as much as possible, while

controlling the number of nonzero loadings in these combinations. In this paper we consider 8 different optimization formulations for computing a single sparse loading vector; these are obtained by combining the following factors: we employ *two* norms for measuring variance (L2, L1) and *two* sparsity-inducing norms (L0, L1), which are used in *two* different ways (constraint, penalty). Three of our formulations, notably the one with L0 constraint and L1 variance, have not been considered in the literature. We give a unifying reformulation which we propose to solve via a natural alternating maximization (AM) method. We show the the AM method is nontrivially equivalent to GPower (Journée et al; JMLR **11**:517–553, 2010) for all our formulations. Besides this, we provide 24 efficient parallel SPCA implementations: 3 codes (multi-core, GPU and cluster) for each of the 8 problems. Parallelism in the methods is aimed at i) speeding up computations (our GPU code can be 100 times faster than an efficient serial code written in C++), ii) obtaining solutions explaining more variance and iii) dealing with big data problems (our cluster code is able to solve a 357 GB problem in about a minute).

Inexact coordinate descent

Rachael Tappenden & Jacek Gondzio & Peter Richtárik *(University of Edinburgh)*

In this work we consider the problem of minimizing a convex composite function using a new randomized block coordinate descent method that uses an "inexact" update. We present convergence guarantees for the algorithm in the form of iteration complexity results. Furthermore, we discuss the use of iterative techniques to determine the inexact update, as well the use of preconditioning for further acceleration.

Applications of domain decomposition to topology optimization

James Turner & Michal Kočvara & Daniel Loghin *(University of Birmingham)*

Topology optimization can be viewed as part of the important branch of computational mechanics known as structural optimization. When modelling such problems, there is a perpetual need for increasingly accurate conceptual designs, with the number of degrees of freedom used in obtaining solutions continually rising. This impacts heavily on the overall computational effort required by a computer and it is therefore natural to consider alternative possibilities. One approach is to consider parallel computing and, in particular, domain decomposition.

In this talk, I will discuss the application of domain decomposition to a typical topology optimization problem via an interior point approach. This method has the potential to be carried out in parallel and can therefore exploit recent developments in the area.

We discuss a novel multilevel approach to Subset Simulation where the failure regions are computed on a hierarchy of finite element meshes. We report numerical experiments with a simple 1D displacement problem and illustrate properties of the new method.

Joint work with Iason Papaioannou (Engineering Risk Analysis Group, TU Mnchen).

Alternating minimization method for matrix completion

Ke Wei *(University of Oxford)*

The problem of recovering a low rank matrix from its partial entries - also known as matrix completion - arises in a wide variety of practical context, such as model reduction, pattern recognition,and machine learning. From the pioneer work of Candes and Recht, the problem has received intensive investigations. Although it is generally a NP-hard problem, there have been many computationally efficient algorithms for it, including the algorithms based on the matrix manifold. In this talk we will present an alternating minimization method and its invariant for matrix completion problem. We will see that how the alternating scheme enables us to take advantage of the sparse structures of the problem, which makes it efficient even as a first order method. Typically it could recover low rank matrix with 10000×10000 by several seconds when OS is around 4. We will compare our algorithms with other solvers, such as, LMaFit [1], LRGeomCG [2], on both random problems and real images. At last, as a non-convex programming, we will show that the limit points of the sequences generated by the algorithm are stationary points.

[1] Z. Wen and W. Yin and Y. Zhang, *Solving A Low-Rank Factorization Model for Matrix Completion by A Nonlinear Successive Over-Relaxation Algorithm.* Mathematical Programming Computation, 2012.
[2] B. Vandereycken, *Low-rank matrix completion by Riemannian optimization.* submitted.

Minisymposium M2

Scientific Software and HPC
Organisers
Timo Betcke and Andreas Dedner

Adapting DUNE's Parallel Algebraic Multigrid to Hybrid Architectures

Markus Blatt *(HPC-Simulation-Software & Services)*

When solving elliptic or parabolic partial differential equations (PDEs) most of the computation time is often spent in solving the arising sparse linear systems. Therefore highly scalable optimal solvers for such systems are mandatory in HPC simulation codes. Besides domain decomposition methods the most scalable and fastest methods are multigrid methods. These can solve sparse linear systems with optimal or nearly optimal complexity, i.e. at most $O(N \log N)$ operations for N unknowns.

In this talk we will investigate the design of the algebraic multigrid (AMG) solver within the "Distributed and Unified Numerics Environment" (DUNE) and its scalability on supercomputers with hundreds of thousands of cores.

Solving sparse linear system is mostly limited by the available memory bandwidth. Based on this fact we discuss possibilities to increase performance and the extension of the method to hybrid architectures. Possible consequences on software design occurring en route will be explored.

A hybrid-algorithm parallelisation approach for the solution of 3D problems

Alessandro Bolis & Spencer J Sherwin *(Imperial College London)*

The fast development of super-computers forces software designers to make a continuous effort to keep algorithms up-to-date and able to exploit all the benefits coming from hardware innovation. In the last decade investigations of numerical schemes, parallelisation paradigms and algorithms efficiency have been fundamental to push the limits forward.

Nektar++ is a C++ library providing support for the solution of partial differential equations using high-order methods. Combining the flexibility of an elemental tessellation with the accuracy of spectral approximations, *Nektar++* is equipped with various algorithmic components to solve 3D problems. A sensible usage of these components can be employed to tune the code to achieve higher levels of parallelism. Parallelisation approaches and numerical discretisation techniques are encapsulated within C++ classes in *Nektar++*. This flexibility facilitates *ad hoc* selections of one or more combined algorithms, allowing the optimised usage of the provided hardware characteristics for the solution of a specific problem. The ability to select the most appropriate numerical method or parallelisation approach plays a relevant role in the parallelisation efficiency portability and, at the same time, provides a solid base for exploiting possible new hardware features. Typical variables characterising a super-computer like latency, bandwidth, cache and available memory per node, can be pushed to their limits selecting the most suitable numerical technique/s. An immediate consequence of this approach is an optimal usage of the computational resources, reducing computational time and costs.

A common scenario in many engineering applications is a 3D problem which needs to be solved with a desired accuracy. Within a 3D spectral/*hp* element discretisation we can can play with various parameters to keep an optimal balance of computations/communications and memory usage. The number of degree of freedoms (*i.e.* the resolution) is proportional to both the number of elements and the spectral expansion order. Proper combinations of these two parameters can maximise the efficiency of a mesh decomposition technique on a given machines, preserving the desired accuracy. Applying a 3D hybrid discretisation (a 2D spectral/*hp* element method combined with a pure spectral discretisation), we can also select which type of parallelisation we want to implement. The parallelisation of the pure spectral expansion generally requires the passage of fewer and bigger messages compared to a mesh decomposition technique. Depending on the hardware features and on the degrees of freedom ratio between the elemental and spectral discretisation, one parallelisation approach may outperform the other. Furthermore, a sensible combination of them could be the most efficient choice and it can be used to amplify the scalability limit.

A practical example of how this philosophy applies to problems of engineering and scientific interest is the DNS of a turbulent flow. Common practice is to gain benefits from a new architecture (larger number of CPUs) increasing the number of degrees of freedom, which allows the investigation of higher Reynolds numbers. Although this weak scalability is still very useful for turbulent simulations, it may not always be of practical interest. We present scalability tests we performed on the Imperial College parallel cluster using *Nektar++*. In these tests we solve the 3D Navier-Stokes equations for two different turbulent flows using the hybrid discretisation method previously mentioned (selecting Fourier as the pure spectral basis). Our studies highlight how the two possible parallel approaches yield to different results in terms of efficiency and scalability. We also show that the combination of these two parallel algorithms allows strong scalability beyond the natural bottlenecks given by the mesh size and the number of Fourier modes.

Explicit methods and HPC : DG for meteorological applications

Andreas Dedner *(University of Warwick)*

In this talk we will introduce a dynamic core for local weather predication based on the Discontinuous Galerkin method. The method is implemented within the Dune software framework (www.dune-project.org). It allows the simulation of the compressible multi species Navier Stokes equations on general 3D meshes in parallel. Special mechanisms are included to allow the simulation of advection dominated ow and for including local grid adaptation. We will demonstrate that the code allows for efficient, highly scalable parallel simulations.

Meteorological simulations are often based on the compressible Euler or Navier- Stokes equations. One important aspect of these schemes is the importance of accu- rately resolving the advective time scales while diffusive time scales (and other fast scales) do not have to be accurately tracked. Therefore some explicit or semi-implicit time stepping scheme is often used. Extra precautions have to be taken to allow these methods to scale to thousands of processors. In this talk some of the approaches we used will be described.

To prove the effectiveness and effciency of our Dune base numerical core, we com- pare it with the dynamical core of the COSMO local area model. COSMO is an operational code, used by many weather services. This comparison was performed in cooperation with the German Weather Service. We compare the performance of the very different cores based on a number of standard meteorological benchmarks.

Investigating the convergence of asynchronous iterative methods

Nick Dingle & Iain Bethune & Mark Bull & Nick Brown & Nicholas Higham & James Hook *(University of Manchester)*

When solving large sparse systems of linear equations in parallel with synchronous iterative techniques, it is necessary to exchange newly-computed vector elements between processors at every iteration. This talk will describe current work on developing and analysing asynchronous iterative algorithms that avoid time consuming synchronous communication operations and thus allow execution to proceed without having to wait for new data to arrive. We present theoretical results supported by practical experimentation.

Tsunami simulation using the OP2 parallel framework

Mike Giles, Endre László, Gihan Mudalige & István Reguly, Serge Guillas, Carlo Bertolli & Paul Kelly *(University of Oxford)*

OP2 is a framework which has been developed at Oxford and Imperial College for the parallel execution of unstructured grid applications on distributed-memory systems using either CPUs or GPUs [1],[2],[3],[4]. The central idea is to separate a high-level specification of an unstructured grid application from the details of its implementation on modern architectures. In this way, an application developer obtains the benefits of simplicity, performance and code longevity, with the OP2 team taking responsibility for the efficient implementation on a variety of multi-core and manycore architectures.

In this talk, we will give an overview of the OP2 API through which a user specifies the application, and the code transformation which is performed automatically to generate CUDA code for execution on NVIDIA GPUs. As an example, we will discuss its use for the parallelisation of the VOLNA tsunami simulation code.

[1] M.B. Giles, G.R. Mudalige, Z. Sharif, G. Markall, and P.H.J. Kelly. Performance analysis and optimisation of the OP2 framework on many-core architectures. *Computer Journal*, 55(2):168–180, 2012.
[2] M.B. Giles, G.R. Mudalige, B. Spencer, C. Bertolli, and I. Reguly. Designing OP2 for GPU architectures. *IEEE Journal of Parallel and Distributed Computing*, online, 2012.
[3] G.R. Mudalige, M.B. Giles, C. Bertolli, and P.H.J. Kelly. Predictive modeling and analysis of OP2 on distributed memory GPU clusters. *ACM SIGMETRICS Performance Evaluation Review*, 40(2):61–67, 2012.
[4] G.R. Mudalige, M.B. Giles, I. Reguly, C. Bertolli, and P.H.J. Kelly. OP2: An active library framework for solving unstructured mesh-based applications on multi-core and many-core architectures. In *Innovative Parallel Computing (InPar '12)*. IEEE, 2012.
[5] D. Dutykh, R. Poncet, and F. Dias. The VOLNA code for the numerical modeling of tsunami waves: Generation, propagation and inundation. *European Journal of Mechanics - B/Fluids*, 30:598–615, 2011.

Energy efficiency aspects of high performance computing for PDEs

Dominik Göddeke *(TU Dortmund)*

Power consumption and energy efficiency are becoming critical aspects in the design and operation of large scale HPC facilities, and it is unanimously recognised that future exascale supercomputers will be strongly

constrained by their power requirements. At current electricity costs, operating an HPC system over its lifetime can already be on par with the initial deployment cost. These power consumption constraints, and the benefits a more energy-efficient HPC platform may have on other societal areas, have motivated the HPC research community to investigate the use of energy-efficient technologies originally developed for the embedded and especially mobile markets. However, lower power does not always mean lower energy consumption, since execution time often also increases. In order to achieve competitive performance, applications then need to efficiently exploit a larger number of processors. In this talk, we discuss how applications can efficiently exploit this new class of low-power architectures to achieve competitive performance. We evaluate if they can benefit from the increased energy efficiency that the architecture is supposed to achieve. The applications that we consider cover three different classes of numerical solution methods for partial differential equations, namely a low-order finite element multigrid solver for huge sparse linear systems of equations, a Lattice-Boltzmann code for fluid simulation, and a high-order spectral element method for acoustic or seismic wave propagation modelling. We evaluate weak and strong scalability on a cluster of 96 ARM Cortex-A9 dual-core processors and demonstrate that the ARM-based cluster can be more efficient in terms of energy to solution when executing the three applications compared to an x86-based reference machine.

Multiscale simulation: an emerging approach for solving complex scientific problems

Derek Groen, James Suter, James Hetherington, Stefan Zasada, Rupert Nash, Miguel Bernabeu & Peter Coveney *(University College London)*

Multiscale simulations are increasingly common in a wide area of scientific disciplines. The concept of having multiple models form a single scientific simulation, with each model operating on its own spatiotemporal scale, gives rise to a range of new challenges. Multiscale simulations often require interdisciplinary scientific expertise to construct, as well as new advances in reliable and accurate model coupling methods, and new approaches in multi-model validation and error assessment. In addition, executing multiscale simulations requires new modes of computing and communication, often involving distributed scenarios where multiple models are required to start simultaneously and intercommunicate at runtime.

In this talk I will reflect on the recent developments in multiscale simulations and modelling, and provide details on how this mode of computing stands apart from many other approaches. I will also present two multiscale problem that we work on at the Centre for Computational Science.

The first problem involves molecular systems of montmorillonite clay and polymers, where we use multiscale parametrization and coarse-graining techniques to investigate the properties of these composite materials. The second simulation involves modelling cerebrovascular blood flow. Here we incorporating input from the wider environment in a cerebrovascular network by coupling a 1D discontinuous Galerkin model to a 3D lattice-Boltzmann model.

Relevant publications include:
Groen et al., accepted by IEEE CiSE: http://arxiv.org/abs/1208.6444
Groen et al., Interface Focus: http://rsfs.royalsocietypublishing.org/content/3/2/20120087.short
Suter et al., MRS 2012: http://journals.cambridge.org/abstract_S1946427412010093

Sparse Communication Avoiding Pivoting

Jonathan Hogg & Jennifer Scott *(STFC Rutherford Appleton Laboratory)*

On future machines communication will be the most expensive operation that algorithms seek to avoid as computation is spread across many cores. Recent developments in dense linear algebra focus on communication avoiding algorithms, particularly for pivoting. However the ideas and methods cannot be ported directly to sparse solvers as their design does not consider fill-in, which still needs to be avoided.

We present a new technique called *subset threshold pivoting* that seeks to extend the traditional sparse threshold pivoting algorithms in a way that reduces the amount of communication required. Two variants are considered: (1) a pessimistic version that guarantees pivoting tests will always be met, and (2) an optimistic heuristic that works most of the time with a back-tracking mechanism for when it gets things wrong.

Boundary-element calculations with BEM++

Wojciech Śmigaj, Simon Arridge, Timo Betcke & Martin Schweiger *(University College London)*

BEM++ (*http://www.bempp.org*) is a general-purpose, open-source C++/Python library for calculations with the boundary element method (BEM), developed since October 2011 at the University College London. It aims to be a high-performance, versatile tool available free of charge for both academic and commercial

purposes.

The upcoming version 2.0 of BEM++ makes it possible to solve the Laplace, Helmholtz and Maxwell equations in three dimensions. Numerical integration is used to evaluate Galerkin discretisations of integral operators defined on surfaces represented with triangular meshes, managed by means of the DUNE library. Discretised operators can be stored as dense matrices or, thanks to an interface to the well-established AHMED library, as $\mathcal{H}$-matrices. The assembly of $\mathcal{H}$-matrices can be done using several variants of the adaptive cross approximation (ACA) algorithm. Users can easily implement custom integral operators. Time-critical operations, such as matrix assembly or $\mathcal{H}$-matrix-vector multiplication, are parallelised for shared-memory machines using Intel Threading Building Blocks.

Objects representing discretised boundary-integral operators implement the abstract linear-operator interface defined by the Thyra module from the Trilinos library. As a result, users of BEM++ have direct access to the wide range of iterative solvers provided by Trilinos. Evaluation of potentials in space (away from object boundary) is supported and, like boundary operator discretisation, can be accelerated with ACA.

A distinguishing feature of BEM++ is its Python interface. Although the core of the library is written in C++, the Python wrappers allow users to rapidly develop BEM codes and easily visualise and postprocess results of their calculations. The goal of scriptability affects the overall design of BEM++, favouring dynamic rather than static polymorphism.

At the conference, we will present the design and current functionality of BEM++ and discuss plans for its further development.

Minisymposium M3

Numerical Analysis Software in Industry

Organisers

Stephen Hendry and Ramaseshan Kannan

Accessible algorithms and usable software

Jon Cherrie & Tanya Morton *(MathWorks)*

When writing software to perform numerical analysis, emphasis is often placed on accuracy and ensuring that the code runs as efficiently as possible. This is not enough for many people. Shared or production code requires a certain amount of functional design from the perspective of the user (scientist, student, software engineer) — if we want people to use our software, we must make it usable. In this talk, I will discuss some design considerations to make complex algorithms more accessible.

Implementing Algorithms for the NAG Library

Edvin Deadman *(NAG Ltd)*

In this talk I will explain how an algorithm goes from pseudocode in an academic paper to a robust and efficient implementation in the NAG Library. I will talk about floating-point arithmetic, accuracy, parallelism and some of the common pitfalls and issues that are encountered when writing numerical software.

Using PLASMA in the NAG library

Joseph Dobson *(NAG Ltd)*

Modern processor architecture requires linear algebra software to have a new algorithmic and software engineering approach to better exploit the ever increasing parallelism. One library taking a novel approach is PLASMA, which implements the functionality of LAPACK using task based parallelism. This talk looks at how we are embedding PLASMA inside the NAG library, a numerical library containing 1700 routines heavily reliant heavily on linear algebra. We will consider the issues that have arisen such as interoperability with other parallel code as well as discussing potential performance gains.

Domain decomposition methods applied to problems in structural analysis

Stephen Hendry *(Arup)*

Methods of domain decomposition are well established in finite element problems, and substructuring in structural problems. In many cases the need for a substructuring approach has reduced as more memory has been available and so direct solutions of the full matrix have been the dominant approach. However with the advance of multi-core processors there is a renewed interest in methods which give a way of splitting the problem into smaller chunks which can be handled in parallel. This paper looks at substructuring and FETI method and their applicability to structural analysis problems. Two particular aspects are considered: the applicability of the methods to static, dynamic and buckling analysis and the scope for reuse of substructures/sub-domains.

Using eigenvectors to detect and fix ill conditioning in structural finite element matrices

Ramaseshan Kannan & Nicholas J. Higham & Françoise Tisseur *(University of Manchester)*

Finite element models in structural engineering can become ill conditioned due to a variety of reasons, including user errors such as modelling oversights or data entry mistakes. The presence of ill conditioning can lead to numerical inaccuracies in structural analysis results. In this work we demonstrate how the eigenvectors of the stiffness matrix have interesting properties that help us identify the cause of ill conditioning and how we use this information as a diagnostic tool. Our technique has been implemented in commercial FE software and we illustrate its efficacy by examples of real life structural models that it was used on.

The effects of plasticity on the condition number of the stiffness matrix

P. Smith, A. Ramage & A.M. Sonnet (*University of Strathclyde)*

In geotechnical finite element analysis, iterative solvers are generally preferred to direct solvers and, for larger problems, iterative solvers provide the only economical way for calculating solutions on a desktop PC. In practice, the speed of convergence of an iterative solver can often be increased dramatically by using a suitable preconditioner. However, the wide range of elasto-plastic constitutive models and the changing nature of the equations during the analysis make effective preconditioning particularly difficult in geotechnical analyses.

Knowledge of the eigenvalue spectrum of the stiffness matrix is helpful in designing effective preconditioners. In this talk, we will study the eigenvalues of the stiffness matrix when the elasto-plastic constitutive matrix is calculated using a Mohr-Coulomb model. In particular, we look at the effect on the condition number of the balance between the elastic and plastic parts of the model. This should provide valuable insight for constructing effective preconditioners.

Minisymposium M4

Numerical Approximation of Wave Propagation Problems

Organisers

Lehel Banjai and Penny Davies

Fast methods for time-domain boundary integral equations

Lehel Banjai, Maryna Kachanovska & Volker Gruhne *(Heriot-Watt University)*

In this talk we will discuss time-domain boundary integral equations for wave propagation and their discretization and fast implementation. The discretization will be done by convolution quadrature in time and by the Galerkin boundary element method in space. The fast implementation will make use of both the sparsity of the resulting matrices and of their Toeplitz structure. Further, the fast multipole method will be used for further savings. Numerical experiments will support the effectiveness of the presented algorithms.

In even dimensions and in the presence of damping (or for visco- and poroelastodynamics) the sparsity is not present in the matrices. We show how techniques created for parabolic equations can be used to overcome the lack of sparsity in these cases.

Solving time-domain wave problems with BEM++

T. Betcke & S. Arridge & J. F.-C. Chan & Y. Guo & P. Monk & W. Śmigaj *(University College London)*

BEM++ (www.bempp.org) is a novel library for the solution of boundary integral formulations of Laplace, Helmholtz and Maxwell problems. The library itself is built on a fast C++ core and offers a convenient Python interface. In this talk we will present the development of a time-domain module for BEM++ based on Convolution Quadrature methods. Performance and parallelisation of the time-domain module will be discussed and several interesting examples for acoustic and electromagnetic problems presented.

Convolution-in-time approximations of time dependent boundary integral equations (TDBIEs)

Dugald B Duncan & Penny J Davies *(Heriot-Watt University)*

We present a new framework for the temporal approximation of TDBIEs which can be combined with either collocation or Galerkin approximation in space. It shares some properties of convolution quadrature, but instead of being based on an underlying ODE solver the approximation is explicitly constructed in terms of basis functions which have compact support, and hence has sparse system matrices.

The time-stepping method is derived as an approximation for convolution Volterra integral equations (VIEs): at time step $t_n = nh$ the VIE solution is approximated in a "backward time" manner in terms of basis functions ϕ_j by $u(t_n - t) \approx \sum_{j=0}^{n} u_{n-j}\phi_j(t/h)$ for $t \in [0, t_n]$. When the basis functions are cubic

B-splines with the "parabolic runout" conditions at $t = 0$ the method is fourth order accurate, and numerical test results indicate that it gives a very stable approximation scheme for acoustic scattering TDBIE problems.

A posteriori error bounds for explicit and implicit methods for the wave equation

M Georgoulis *(University of Leicester)*

The class of second degree cosine methods, also known as the Newmark family of numerical methods for wave problems is used extensively in practical computations. This family includes the very popular explicit leap-frog method for a particular choice of method parameters. This work is concerned with the derivation of optimal order a posteriori error bounds for time-discretizations based on second degree cosine methods. A key argument is a carefully selected perturbation of the original leapfrog method, retaining the optimal order of convergence, while simultaneously allowing for second order time-reconstructions, thereby retaining the order of the method. This is based on joint work with O. Lakkis (Sussex) and Ch. Makridakis (Crete).

Hybrid numerical-asymptotic approximation for high frequency scattering by penetrable convex polygons

Samuel Groth & David Hewett & Stephen Langdon *(University of Reading)*

We consider the two-dimensional problem of scattering of a time-harmonic wave by a penetrable convex polygon Ω with boundary $\partial\Omega$. We wish to determine the total field u_1 in the exterior domain D and the total field u_2 within the polygon such that

$$\Delta u_1 + k_1^2 u_1 = 0, \quad \text{in } D, \tag{1}$$

$$\Delta u_2 + k_2^2 u_2 = 0, \quad \text{in } \Omega, \tag{2}$$

$$u_1 = u_2 \text{ and } \frac{\partial u_1}{\partial \mathbf{n}} = \frac{\partial u_2}{\partial \mathbf{n}}, \quad \text{on } \partial\Omega, \tag{3}$$

where $k_1, k_2 \in \mathbb{C}$ are the wavenumbers in D and Ω, respectively, with $\mathrm{Re}(k_1), \mathrm{Re}(k_1) > 0$ and $\mathrm{Im}(k_1), \mathrm{Im}(k_2) > 0$, and $\mathbf{n}$ denotes the unit vector normal to $\partial\Omega$ directed into D.

Standard numerical methods for scattering problems, using piecewise polynomial approximation spaces, require a fixed number of degrees of freedom per wavelength in order to represent the oscillatory solution. This leads to prohibitive computational expense in the high frequency regime. For problems of scattering by *impenetrable* scatterers, where there is just one wavenumber k, much work has been done on developing and analysing *hybrid numerical-asymptotic* (HNA) methods (see [1]) which overcome this limitation. These HNA methods approximate the unknown boundary data v in a *boundary element method* framework using an ansatz of the form

$$v(\mathbf{x}, k) \approx v_0(\mathbf{x}, k) + \sum_{m=1}^{M} v_m(\mathbf{x}, k) \exp(\mathbf{i}k\psi_m(\mathbf{x})), \quad \mathbf{x} \in \Omega, \tag{4}$$

where the phases ψ_m are chosen using knowledge of the high frequency asymptotics. The expectation is that if v_0 (the geometric optics) and ψ_m are chosen well, then v_m will be much less oscillatory than v and so can be more efficiently approximated by piecewise polynomials than v itself.

This talk discusses the challenging task of generalising the HNA methodology to so-called "transmission problems" involving *penetrable* scatterers, as in (1)–(**??**). The main difficulty in this generalisation is that the high frequency asymptotic behaviour is significantly more complicated than for the impenetrable case. In particular, the boundary of the scatterer represents an interface between two media with different wavenumbers, and so we expect to need to modify the ansatz (4) to include terms oscillating at both wavenumbers.

We discuss how appropriate phases are chosen in the penetrable case using high frequency asymptotics and hence show how effective HNA approximation spaces can be constructed for this problem. Moreover, we demonstrate, via comparison with a reference solution, that these HNA approximation spaces can approximate the highly oscillatory solution of the transmission problem accurately and efficiently at all frequencies. Full details can be found in [2].

[1] S. N. Chandler-Wilde, I. G. Graham, S. Langdon and E. A. Spence, *Numerical-asymptotic boundary integral methods in high-frequency acoustic scattering*, Acta Numerica (2012),
pp. 89–305.
[2] S. P. Groth, D. P. Hewett and S. Langdon, *Hybrid numerical-asymptotic approximation for high frequency scattering by penetrable convex polygons*, submitted for publication, University of Reading preprint MPS-2013-02.

Locally enriched finite element method for 3D elastic wave problems

O. Laghrouche & M. S. Mahmood & & A. El-Kacimi & J. Trevelyan *(Heriot-Watt University)*

Our aim is to develop finite elements, for three di-

mensional elastic wave problems, capable of containing many wavelengths per nodal spacing.

In the current work, the concept of the PUFEM for 2D [1],[2] will be extended to the three dimensional time-harmonic elastic wave model. To the authors' knowledge, only very few work have addressed the enrichment approximation in context of 3D elastic wave problem. Generally, the displacement field in 3D is approximated also via the superimposing horizontal (P-wave) and vertical (S-wave) displacements. This decomposition is expanded using plane wave basis functions, corresponding to these displacements, with respect to many directions. However, the crucial differences of 3D in comparison to 2d are: Even though in (2D) there is only one orthogonal vector associated to each component of the vertical displacement(S-wave), in (3D) it is required two orthogonal vectors, to the horizontal vector, for each component to capture the vertical displacement. Furthermore, in two dimensions the directions are easy to calculated whether in uniform or nonuniform distribution, this is not the case in three dimensional problem. Then the issue that raises here is how to generate uniform and nonuniform directions. Here, the focus is set on the uniform case. For this purpose a simple approach depend on the cubic distribution has been explored to generate a relatively uniform directions.

Such approach will allow us to relax the traditional requirement of around ten nodal points per wavelength and therefore solve elastic wave problems without refining the mesh of the computational domain at each frequency. The accuracy and effectiveness of the proposed technique will be determined by comparing solutions for selected problems with available analytical solutions and/or to high resolution numerical solutions using conventional finite elements.

[1] El Kacimi A and Laghrouche O. Numerical Modelling of Elastic Wave propagation in Frequency Domain by the Partition of Unity Finite Element Method. International Journal for Numerical Methods in Engineering, 77: 1646-1669, 2009.
[2] El Kacimi A and Laghrouche O. Improvement of PUFEM for the numerical solution of high frequency elastic wave scattering on unstructured triangular mesh grids. International Journal for Numerical Methods in Engineering, 84: 330-350, 2010.

A modified spectral element method for efficient time-stepping for the acoustic wave equation

Mark Payne *(Heriot-Watt University)*

The Spectral Element Method, a Finite Element formulation designed for time dependent wave problems, produces a diagonal mass matrix which eliminates the need for linear solvers at each time step. To obtain higher order accuracy in time it is normal for schemes such as the modified equation approach to be used. However, these approaches involve the multiple application of the spatial matrix operator which increases the time per time step.

In this talk we introduce the formulation of an improved method which maintains accuracy at main node points with only one application of the spatial matrix operator. By focusing on only the accuracy at the main node points we can eliminate the sub-nodes to produce a multi-level finite difference scheme, through analysis of which we can find coefficients which cancel the errors between time and space discretisations and so produce Spectral Element like schemes with only one spatial operator application.

Shifted Laplace DDM preconditioners for the Helmholtz equation

J. D. Shanks, P.N. Childs & I.G. Graham *(University of Bath)*

We consider iterative methods for solving the Helmholtz equation with motivation coming from applications in seismic imaging. When solving the Helmholtz equation on an infinite domain, one can consider as a model problem the following boundary value problem on a finite domain Ω,

$$\begin{aligned} -\Delta u - k^2 u &= f, \text{ in } \Omega \subset \mathbb{R}^d, \text{ for } d = 2, 3, \\ \left(\frac{\partial}{\partial n} - ik\right) u &= 0, \text{ on } \partial\Omega, \end{aligned} \tag{5}$$

where k is the wavenumber, f is some source, $\frac{\partial}{\partial n}$ denotes the normal derivative, and where the impedance condition on $\partial\Omega$ is an approximation of the exact far field condition. Once this is discretised with finite elements, we solve the linear system $A\mathbf{U} = f$, where the matrix A is complex, symmertric but highly non-Hermitian. Because of the latter property, conventional iterative methods can fail to converge so it is necessary to precondition the linear system before solving using an iterative method such as GMRES. Some recent research has focused on preconditioning this system with the discretisation of the following complex shifted problem,

$$\begin{aligned} -\Delta u - \left(k^2 + i\epsilon\right) u &= f, \text{ in } \Omega \subset \mathbb{R}^d, \text{ for } d = 2, 3, \\ \left(\partial_n - i\sqrt{k^2 + i\epsilon}\right) u &= 0, \text{ on } \partial\Omega, \end{aligned} \tag{6}$$

which we shall call $A_\epsilon \mathbf{U} = f$. This idea was used by Erlangga and others used solves with the Restricted Additive Schwarz method to approximate A_ϵ^{-1}. The

choice of ϵ so that A_ϵ is a good preconditioner for A and also so that iterative methods for approximating A_ϵ^{-1} work well is a delicate business. In this talk we will discuss an optimised Schwarz domain decomposition algorithm for this problem. This can also be used as a preconditioner for the original Helmholtz equation. An analysis of the algorithm will be presented along with numerical results.

Is the Helmholtz equation really sign-indefinite?

Euan A. Spence & Andrea Moiola *(University of Bath)*

The usual variational (or weak) formulations of the Helmholtz equation are sign-indefinite in the sense that the bilinear forms cannot be bounded below by a positive multiple of the appropriate norm squared. This is often for a good reason, since in bounded domains under certain boundary conditions the solution of the Helmholtz equation is not unique at certain wavenumbers (those that correspond to eigenvalues of the Laplacian), and thus the variational problem cannot be sign-definite. However, even in cases where the solution is unique for all wavenumbers, the standard variational formulations of the Helmholtz equation are still indefinite when the wavenumber is large. This indefiniteness has implications for both the analysis and the practical implementation of finite element methods.

In this talk I will discuss new *sign-definite* (also called *coercive* or *elliptic*) formulations of the Helmholtz equation posed in either the interior of a star-shaped domain with impedance boundary conditions, or the exterior of a star-shaped domain with Dirichlet boundary conditions. Like the standard variational formulations, these new formulations arise just by multiplying the Helmholtz equation by particular test functions and integrating by parts.

B-spline FEM approximation of wave equation

Hongrui Wang & Mark Ainsworth *(University of Strathclyde)*

The use of high order splines for the approximation of PDEs has recently attracted a lot of attention due to the work of Hughes [1]. However, it is as yet unclear how these methods perform as the order of approximation is increased on a fixed mesh. We analyse this problem in the setting of the wave equation and present rigorous convergence results. We also show how the methods can be implemented efficiently and analyse their stability.

[1] John A. Evans, Yuri Bazilevs, Ivo Babuska, and Thomas J.R. Hughes. N-widths, sup-infs, and optimality ratios for the k-version of the isogeometric finite element method. *Computer Methods in Applied Mechanics and Engineering*, 198:1726 – 1741, 2009.

Minisymposium M5

Numerical Methods for Layer Phenomena

Organiser: Torsten Linß

Linear Finite Elements may be only First-Order Pointwise Accurate on Anisotropic Triangulations

Natalia Kopteva *(University of Limerick)*

It appears that there is a perception in the finite-element community that the computed-solution error in the maximum norm is closely related to the corresponding interpolation error.

While an almost best approximation property of finite-element solutions in the maximum norm has been rigourously proved (with a logarithmic factor in the case of linear elements) for some equations on quasi-uniform meshes, there is no such result for strongly-anisotropic triangulations. Nevertheless, this perception is frequently considered a reasonable heuristic conjecture to be used in the anisotropic mesh adaptation.

In this talk, we give a *counterexample* of an *anisotropic triangulation* on which

- the exact solution is in $C^\infty(\bar{\Omega})$ and has a second-order pointwise error of linear interpolation $O(N^{-2})$,
- the computed solution obtained using linear finite elements is only first-order pointwise accurate, i.e. the pointwise error is as large as $O(N^{-1})$.

Here the maximum side length of mesh elements is $O(N^{-1})$ and the global number of mesh nodes does not exceed $O(N^2)$.

Our example is given in the context of a singularly perturbed *reaction-diffusion* equation, whose exact solution exhibits a sharp boundary layer. Both standard and lumped-mass cases are addressed. A theoretical justification of the observed numerical phenomena is given by the following lemma (which is established using a finite-difference representation of the considered finite element methods).

Suppose $\Omega \supset \mathring{\Omega}$, where the subdomain $\mathring{\Omega} := (0, 2\varepsilon) \times$

$(-H, H)$ with the tensor-product mesh $\{x_i = \varepsilon \frac{i}{N_0}\}_{i=0}^{2N_0} \times \{-H, 0, H\}$. Various triangulations $\mathring{\mathcal{T}}$ in $\mathring{\Omega}$ can be obtained by drawing diagonals in each rectangle (as for each rectangle $ABCD$ one can use either the diagonal AC or BD).

Lemma. *Let $u = e^{-x/\varepsilon}$ be the exact solution of the equation $-\varepsilon^2 \triangle u + u = 0$, subject to a Dirichlet boundary condition, posed in a domain $\Omega \supset \mathring{\Omega}$, a triangulation $\mathcal{T}$ in Ω be such that $\mathcal{T} \supset \mathring{\mathcal{T}}$, and U be the computed solution obtained using linear finite elements. For any positive constant C_2, there exist a triangulation $\mathring{\mathcal{T}}$ and sufficiently small constants C_0 and C_1 such that if $N_0^{-1} \le C_1$ and $\varepsilon \le C_2 H$, then*

$$\max_{\bar{\Omega}} |U - u| \ge C_0 N_0^{-1}.$$

Similar phenomena will be also discussed in the context of singularly perturbed *convection-diffusion* equations.

Maximum-norm a posteriori error estimates for parabolic equations

Torsten Linß & Natalia Kopteva *(Fern Universiät)*

For classical and singularly perturbed 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 discretised in time using the backward Euler method, the Crank-Nicolson method and the discontinuous Galerkin dG(r) method. Both semidiscrete (no spatial discretation) and fully discrete cases will be considered. The analysis is based on elliptic reconsturcions and elliptic a posteriori error estimates.

A boundary layer preconditioner for a singularly perturbed problem

Niall Madden & Scott MacLachlan *(NUI Galway)*

We consider the problem of computing numerical solutions to a singular perturbed two-dimensional reaction-diffusion problems posed on the unit square. Using a finite difference scheme on a layer adapted mesh, one can obtain an approximation for which the associated error bound depends only on the discretization parameter, N, and not on the perturbation parameter, ε. Of course this process also requires that a linear system of equations be solved. We investigate if this can be done in a way that is robust with respect to the perturbation parameter.

It has been shown that, surprisingly, standard direct solvers exhibit poor scaling behaviour when solving the resulting linear systems. We consider, instead, a new block-structured preconditioning approach, and compare its efficiency with some standard multigrid preconditioners.

Pointwise accuracy of numerical approximations to the scaled partial derivatives of the solutions to singularly perturbed elliptic problems.

E. O'Riordan & J. L. Gracia *(Dublin City University)*

The solutions of singularly perturbed problems typically contain steep gradiants in narrow regions of the domain, often referred to as layer regions. Layer adapted meshes, such as piecewise-uniform Shishkin meshes or Bakhvalov meshes, have been designed to concentrate a significant proportion of the mesh points into these layer regions and thereby generate pointwise globally accurate piecewise–polynomial approximations to the continuous solution, irrespective of the size of the singular perturbation parameter. An additional feature of these layer-adapted meshes is that accurate approximations to the first derivative of the solution can be easily generated. For a singularly perturbed elliptic partial differential equation of convection-diffusion type, we discuss some issues related to the appropriate scaling of the first order derivatives and outline a proof of the parameter-uniform convergence of the discrete partial derivatives for a numerical method consisting of an upwinded finite difference operator on a piecewise-uniform Shishkin mesh.

Experiments with a Shishkin Algorithm for a Singularly Perturbed Quasilinear Parabolic Problem with a Moving Interior Layer.

Jason Quinn *(Dublin City University)*

In [G.I. Shishkin, Difference Approximation of the Dirichlet Problem for a Singularly Perturbed Quasilinear Parabolic Equation in the Presence of a Transition Layer, *Russian Acad. Sci. Dokl. Math.*, (1994) **48**(2) 346-352.], Shishkin presented and analysed a numerical method for the following type of singularly perturbed parabolic problem

$$(\varepsilon u_{xx} - u u_x - b u - u_t)(x,t) = f(x,t),$$

$$(x,t) \in G := (-1,1) \times (0,T]$$

$$b(x,t) \ge 0, \ (x,t) \in \bar{G}, \quad u(x,t) = \phi(x,t), \ (x,t) \in \bar{G} \backslash G,$$

$$\phi(0,t) > 0, \quad \phi(1,t) < 0, \quad \phi(d,0) = 0, \quad \phi = \phi_0 + \phi_1,$$

$$\|\phi_0{}'\| \le C, \ \ |\frac{\partial^k}{\partial x^k} \phi_1(x,t)| \le C \varepsilon^{-k} e^{-C_1 |d-x|/\varepsilon},$$

$$1 \le k \le 5, \quad (x,t) \in \bar{G} \setminus G.$$

We implement this method and present numerical results to illustrate the convergence properties of the method in practice.

Convergence in balanced norms for reaction-diffusion problems

Martin Schopf & Hans-Görg Roos, *(Technical University of Dresden)*

Error estimates of finite element methods for reaction-diffusion problems are often realized in the related energy norm. In the singularly perturbed case, however, this norm is not adequate: It is too weak to capture the boundary layers. The multiplier of its H^1 seminorm component is too small. We refer to this norm as unbalanced since different components of it have different orders of magnitude.

A different scaling of the H^1 seminorm leads to a balanced and stronger norm. This one reflects the layer behaviour correctly. We give a survey on methods providing error estimates in balanced norms and show how these can be obtained for the Galerkin finite element method.

A priori bounds for a variable-coefficient elliptic convection-diffusion problem

Martin Stynes & Natalia Kopteva *(National University of Ireland, Cork)*

In the two papers

- Corner singularities and boundary layers in a simple convection-diffusion problem, J. Differential Equations 213 (2005), no. 1, pp.81-120
- Sharpened bounds for corner singularities and boundary layers in a simple convection-diffusion problem, Appl. Math. Lett. 20 (2007), no. 5, pp.539-544

Kellogg and Stynes derived pointwise bounds on the derivatives of solutions to a convection-diffusion problem posed on the unit square, where the differential operator was of constant-coefficient type and the data satisfied an arbitrary number of compatibility conditions at the corners of the domain. These bounds gave precise information about the interactions between boundary layers (caused by the singularly perturbed nature of the problem) and corner singularities (caused by corner incompatibilities in the data), and were used subsequently by various researchers in the numerical analysis of finite difference and finite element methods for this class of problems.

In this talk, a critical aspect of the extension of these results to convection-diffusion operators with *variable* coefficients will be discussed.

Minisymposium M6

Fast and Accurate Uncertainty Quantification

Organisers

Catherine Powell and Rob Scheichl

Fast and accurate uncertainty quantification (UQ)

Sondipon Adhikari *(Swansea University)*

The study of numerical methods for solving PDEs with deterministic data is mature in many application areas. Recently, there has been an explosion of research into numerical methods for solving PDEs with uncertain data. Such data is often modelled as stochastic processes or random fields and we look to numerical methods that quantify the uncertainty in the solution, given a statistical model for the data. Until recently, most of this research has focused on the model elliptic problem, with random coefficients. Now, also more interesting PDE problems e.g. the Navier-Stokes equations, are starting to be tackled.

Techniques such as Monte Carlo methods, stochastic Galerkin methods and stochastic collocation methods, lead to interesting and extremely challenging linear algebra problems. Sampling methods ultimately lead to a sequence of systems (often many thousands, or even hundreds of thousands) with the dimension of a deterministic problem. The challenge lies not only in exploiting the obvious levels of parallelism, but also the similarity of the systems. On the other hand, projection schemes like stochastic Galerkin methods, which often have superior convergence properties, couple deterministic and stochastic degrees of freedom, and require the solution of an extremely large matrix system. Such matrices are usually highly structured. Here, the challenge lies in solving the system without assembling it, by exploiting the Kronecker product structure and again exploiting (less obvious) levels of parallelism. This mini-symposium focuses on efficient linear algebra, fast solvers and preconditioners in UQ studies of a range of PDEs and systems of PDEs.

Convergence analysis for multilevel variance estimators in Multilevel Monte Carlo Methods and application for random obstacle problems

Alexey Chernov & Claudio Bierig *(University of Bonn)*

The Multilevel Monte Carlo Method (MLMC) is a re-

cently established sampling approach for uncertainty propagation for problems with random parameters. Under certain assumptions, MLMC allows to estimate e.g. the mean solution and k-point correlation functions at essentially the same overall computational cost as the cost required for solution of one forward problem for a fixed deterministic set of parameters.

However, in many practical applications estimation of the variance (along with the mean) is the main goal of the computations. In this case the variance can be potentially computed from correlation functions in the post-processing step. This approach has two drawbacks:

1. Optimal complexity approximation of correlation functions involves quite cumbersome sparse tensor product constructions. It is desirable to avoid it if the variance is the aim of the computation.

2. Computation of the variance from the 2-point correlation function is prone to numerical instability, specially in the case of small variances.

Much less is known about direct estimation of the variance, potentially overcoming these difficulties. In this talk we present new convergence theorems for the multilevel variance estimators. As a result, we prove that under certain assumptions on the parameters, the variance can be estimated at essentially the same cost as the mean, and consequently as the cost required for solution of one forward problem for a fixed deterministic set of parameters. We comment on fast and stable evaluation of the estimators suitable for parallel large scale computations.

The suggested approach is applied to a class of scalar random obstacle problems, a prototype of contact between deformable bodies. In particular, we are interested in rough random obstacles modelling contact between car tires and variable road surfaces. Numerical experiments support and complete the theoretical analysis.

A Bayesian Approach to Shape Registration

Simon Cotter & Colin Cotter & F.-X. Viallard *(University of Manchester)*

With the advent of more advanced prenatal scanning technologies, there is a need for diagnostic tools for certain congenital conditions. This problem amounts to finding the distance in shape space between a noisily observed scan of a particular organ, be it brain or heart etc, and a library of shapes of organs from babies that had particular conditions.

We frame the problem as a Bayesian inverse problem on function space, where the functions of interest relate to the geodesic flow fields that deform one shape into the other. This is analogous to finding the velocity field in a Lagrangian data assimilation problem. Using regularity results regarding the forward problem, we identify minimal-regularity priors in order to make the inverse problem well-posed. We then present some numerics for simple 2D examples on closed curves, which show how the posterior distributions on function space can be sampled using MCMC methods. This allows us to estimate the distance in shape space between the two objects, and to quantify the uncertainty in that estimation.

Variational Smoothing Filters for Sequential Inverse Problems

Chris Farmer *(University of Oxford)*

Given a system model, a model of any measuring apparatus that relates states to observations, and a prior assessment of uncertainty, the probability density of subsequent system states, conditioned upon the history of the observations is a logical consequence of the models and the values of the observations.

When observations are made at discrete times, it is known that the evolving probability density is a solution of the Bayesian filtering equations. This talk will examine the consequences of seeking to approximate the evolving probability density using a Gaussian mixture (i.e. a sum of Gaussian densities). In general this leads to a sequence of optimisation problems and related high-dimensional integrals. There are other problems too, related to the necessity of using a small number of densities in the mixture, the requirement to maintain sparsity of any matrices and the need to compute first and, somewhat disturbingly, second derivatives of the misfit between predictions and observations. Adjoint methods, Taylor expansions, Gaussian random fields and Newton's method can be combined to, possibly, provide a solution. This approach is essentially a combination of filtering methods and '4-D Var' methods.

Some progress has now been made which will be explained, and the remaining severe difficulties described. The generalised Lorenz-96 equations, where in addition to the variables, many unknown parameters are also present, will be used as an example. Results will be presented that indicate that when the equations are correct and the uncertainty is quantified with sufficient accuracy, one can retrieve (i) an estimate of the variables with very few observations upon them and (ii) a posterior density for the variables and parameters which has lower uncertainty than at the start of

the process. One is led to conjecture that the near optimal solution of an inverse problem, when performed in a Bayesian setting, contains much valuable information that is usually missed.

Quasi-Monte Carlo finite element methods for elliptic PDEs with log-normal random coefficients

Ivan G. Graham *(University of Bath)*

In this talk we describe quasi-Monte Carlo (QMC) methods for computing the expectations of functionals of solutions of elliptic PDEs, with coefficients defined as log-normal Gaussian random fields. As we see, these methods outperform conventional Monte Carlo methods for such problems. Our main target application is the computation of several quantities of physical interest arising in the modeling of fluid flow in random porous media, such as the effective permeability or the exit time of a plume of pollutants. Such quantities are of great interest in uncertainty quantification in areas such as underground waste disposal.

There is considerable practical interest in the case of relatively high variance and low correlation length, leading to high stochastic dimension. In this case Monte Carlo is currently the method of choice but, as we demonstrate, QMC methods are more effective and efficient for a range of parameters and quantities of interest.

We will briefly describe a practical algorithm [1], including some numerical results involving very high dimensions. Then we will give an overview of some recent theoretical advances [2] which in particular identify circumstances under which the convergence of the QMC method is independent of stochastic dimension.

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[2] I.G. Graham, F.Y. Kuo, J.A. Nichols, R. Scheichl, Ch Schwab and I.H. Slona, Quasi-Monte Carlo finite element methods for elliptic PDEs with log-normal random coefficients, submitted.

Evaluation of Gaussian approximations to Bayesian inverse problems in subsurface models

Marco A. Iglesias & Kody J.H. Law and Andrew Stuart *(University of Warwick)*

We discuss the numerical evaluation of Gaussian approximations to the posterior distribution that arises in Bayesian data assimilation for reservoir characterization. In particular, we evaluate (i) linearization around the maximum a posterior estimate, (ii) randomized maximum likelihood, (iii) ensemble Kalman filter and its variants (e.g. square root filter and localization). For our evaluation, we use a state-of-the art Markov Chain Monte Carlo (MCMC) method to accurately characterize the posterior distribution of the log-permeability conditioned to dynamic data. Therefore, MCMC provides a gold standard against which to compare the performance of the Gaussian approximations in terms of mean and variance. Our evaluations are performed on 2D synthetic experiments with relevant prototypical reservoir models.

Stochastic Finite Element Method for dynamical systems with random boundary topology

Abhishek Kundu *(Swansea University)*

Random boundary topology is an important source of uncertainty in many computational mechanics problems. This might occur due to lack of control in manufacturing process, insufficient data, measurement errors or a combination of these factors. They become significant in problems which are sensitive to boundary topology (such as high speed flow problems or future generation of structural materials for advanced applications). On the other hand, parametric uncertainty in material properties is another source of randomness and have been dealt with significant rigor and generality within the scope of classical stochastic finite element analysis. However, the consideration of geometric uncertainty expressed as domain boundaries within a computational mechanics framework has received rather less attention. Surface roughness has been quantified in various fields using methods ranging from simple parametrization of surface inhomogeneities to using fractals for representing the perturbations in the domain. Here we have chosen the random field model to quantify the uncertainty in boundary topology. The aim of this work is to integrate the treatment of parametric and boundary uncertainties in a generic fashion within a stochastic spectral finite element method.

A discrete version of Karhunen-Loève Expansion is proposed here which utilizes finite element nodal points to expand the random field with a set of orthogonal spatial basis functions and a finite order chaos expansion. The truncated random field representation has been incorporated within the stochastic weak formulation and applied to probabilistic mechanics problems with random parameters and boundary conditions. Random boundary topology leads to the necessity of using stochastic shape functions in a tensor product space. The random Jacobian matrix which maps the

elements in the FE mesh to its master element, gives rise to non-linear stochastic functions. This has been tackled within the framework of stochastic spectral Galerkin method. A-posteriori error estimation has been performed to highlight the convergence behavior of the discretized mathematical model with the order and dimension of the stochastic and spatial shape functions respectively. The study demonstrates an efficient scheme of tackling boundary uncertainty in general irregular domain with a variety of covariance function descriptions of the random field.

Low Rank Solution of Unsteady Diffusion Equation with Stochastic Coefficients

A. Onwunta, M. Stoll and P. Benner *(Max Planck Institute for Dynamics of Complex Technical Systems)*

We study the solution of linear systems resulting from the discreitization of unsteady diffusion equation with stochastic coefficients. In particular, we focus on those systems that are obtained using the so-called stochastic Galerkin finite element method (SGFEM). These systems are usually very large with Kronecker product structure and, thus, solving them can be both time- and computer memory-consuming. Under certain assumptions, we show that the solution of such linear systems can be approximated with a vector of low tensor rank. We then solve the linear systems using low rank preconditioned iterative solvers. Numerical experiments demonstrate that these low rank preconditioned solvers save time and computer memory.

A new variance reduction technique for multilevel Monte Carlo methods
coarse grid variates

Minho Park, Andrew Cliffe & Mike Giles *(University of Nottingham)*,

Multilevel Monte Carlo (MLMC) methods have been used in a range of stochastic differential equation applications. The merit of MLMC is that it can achieve the same asymptotic cost for stochastic problems as for deterministic problems. However, a larger constant in the estimate for the computational complexity is generally required.

In this talk we introduce a new and effective variance reduction technique, called coarse grid variates (CGV), to be used to improve the MLMC convergence. We then present numerical results showing the combination of MLMC and CGV can achieve the same accuracy of results at substantially smaller computational cost. Moreover, we will also address how to extend this technique to the realisations conditioned on observed data.

Efficient Solvers for Steady-State Navier–Stokes Equations with Random Data

Catherine E. Powell & David Silvester *(University of Manchester)*

We consider the numerical solution of the steady-state Navier–Stokes equations with uncertain data. Specifically, we treat the case of uncertain viscosity, which results in a flow with an uncertain Reynolds number. After linearization, we apply a stochastic Galerkin mixed finite element method, combining standard inf-sup stable Taylor–Hood approximation on the spatial domain with orthogonal polynomials in the stochastic parameter. This yields a sequence of non-symmetric saddle-point problems with Kronecker product structure.

Using existing deterministic software, based on the so-called Pressure Convection-Diffusion and Least-Squares Commutator approximations, we introduce efficient block triangular preconditioners for the discrete systems. Theoretical analysis reveals that the preconditioners are robust with respect to the discretization and statistical parameters and numerical results are presented for standard test problems. These include 'flow over a backward-facing step' and 'flow around an obstacle', which require highly stretched grids on the spatial domain.

Multilevel Markov Chain Monte Carlo with Applications in Subsurface Flow

Robert Scheichl, C. Ketelsen & A.L. Teckentrup *(University of Bath)*

One of the key tasks in many areas of subsurface flow, most notably in radioactive waste disposal and oil recovery, is an efficient treatment of data uncertainties and the quantification of how these uncertainties propagate through the system. Similar questions arise also in other areas of science and engineering such as weather and climate prediction or manufacturing. The mathematical challenge associated with these questions is the solution of high-dimensional quadrature problems with integrands that involve the solution of PDEs with random coefficients. Due to the heterogeneity of the subsurface and the complexity of the flow, each realisation of the integrand is very costly and so it is paramount to make existing uncertainty quantification tools more efficient. Recent advances in Monte Carlo type methods, based on deterministic, Quasi–Monte Carlo sampling rules and multilevel approaches, provide unprecedented opportunities for accurate uncertainty analyses in realistic three-dimensional subsurface flow applications. In this talk we show how the multilevel framework can also be ex-

tended to Monte Carlo Markov chain (MCMC) methods, allowing for uncertainty reduction by conditioning on measured data via Bayesian techniques. In particular, we present a multilevel Metropolis-Hastings algorithm including a complete analysis. As in the earlier work, the analysis reduces to classical questions in regularity and finite element approximation error analysis. We can show significant gains over the standard Metropolis-Hastings estimator for a typical model problem in subsurface flow. Numerical experiments confirm the analysis and demonstrate the effectiveness of the method with consistent reductions of a factor of $\mathcal{O}(10-50)$ in the ε-cost for tolerances ε around 10^{-3}.

A posteriori error estimation for stochastic Galerkin approximation

David Silvester & Alex Bespalov & Catherine Powell *(University of Manchester)*

Stochastic Galerkin finite element approximation is an increasingly popular approach for the solution of elliptic PDE problems with correlated random data. Given a parametrisation of the data in terms of a large, possibly infinite, number of random variables, this approach allows the original PDE problem to be reformulated as a parametric, deterministic PDE on a parameter space of high, possibly infinite, dimension. A typical strategy is to combine conventional (h-) finite element approximation on the spatial domain with spectral (p-) approximation on a finite-dimensional manifold in the (stochastic) parameter space.

For approximations relying on low-dimensional manifolds in the parameter space, stochastic Galerkin finite element methods have superior convergence properties to standard sampling techniques. On the other hand, the desire to incorporate more and more parameters (random variables) together with the need to use high-order polynomial approximations in these parameters inevitably generates very high-dimensional discretised systems. This in turn means that adaptive algorithms are needed to efficiently construct approximations, and fast and robust linear algebra techniques are essential for solving the discretised problems.

Both strands will be discussed in the talk. We outline the issues involved in a posteriori error analysis of computed solutions and present a practical a posteriori estimator for the approximation error. We introduce a novel energy error estimator that uses a parameter-free part of the underlying differential operator—this effectively exploits the tensor product structure of the approximation space and simplifies the linear algebra. We prove that our error estimator is reliable and efficient. We also discuss different strategies for enriching the discrete space and establish two-sided estimates of the error reduction for the corresponding enhanced approximations. These give computable estimates of the error reduction that depend only on the problem data and the original approximation. We show numerically that these estimates can be used to choose the enrichment strategy that reduces the error most efficiently.

Multi Level Monte Carlo methods with Control Variate for elliptic SPDEs

F. Tesei & F. Nobile, E. von Schwerin, R. Tempone *(EPF de Lausanne)*

We consider the numerical approximation of a partial differential equation (PDE) with random coefficients. Nowadays such problems can be found in many applications in which the lack of available measurements make an accurate reconstruction of the coefficients involved in the mathematical model unfeasible. In particular we focus on a model problem given by an elliptic partial differential equation in which the randomness is given by the diffusion coefficient, modeled as a random field with limited spatial regularity. This approach is inspired by the groundwater flow problem which has a great importance in hydrology: in this context the diffusion coefficient is given by the permeability of the subsoil and it is often modeled as a lognormal random field. Several models have been proposed in the literature leading to realizations having varying spatial smoothness for the covariance functions. In particular, a widely used covariance model is the exponential one that has realizations with Hölder continuity $\mathcal{C}^{0,\alpha}$ with $\alpha < \frac{1}{2}$.

Models with low spatial smoothness pose great numerical challenges. The first step of their numerical approximation consists in building a series expansion of the input coefficient; we use here a Fourier expansion; whenever the random field has low regularity, such expansions converge very slowly and this makes the use of deterministic methods such as Stochastic Collocation on sparse grids highly problematic since it is not possible to parametrize the problem with a relatively small number of random variables without a significant loss of accuracy. A natural choice is to try to solve such problems with a Monte Carlo type method. On the other hand it is well known that the convergence rate of the standard Monte Carlo method is quite slow, making it impractical to obtain an accurate solution since the associated computational cost is given by the number of samples of the random field multiplied by the cost needed to solve a single deterministic PDE which require a very fine mesh due to the roughness of the coefficient. Multilevel Monte Carlo methods have already been proposed in the lit-

erature in order to reduce the variance of the Monte Carlo estimator, and consequently reduce the number of solves on the fine grid.

In this work we propose to use a multilevel Monte Carlo approach combined with an additional control variate variance reduction technique on each level in order to solve the elliptic SPDE for different choices of the covariance function of the input field characterized by different regularities. The control variate is obtained as the solution of the PDE with a regularized version of the lognormal random field as input random data and its mean can be successfully computed with a Stochastic Collocation method on each level. The solutions of this regularized problem turn out to be highly positively correlated with the solutions of the original problem.

Within this Monte Carlo framework the choice of a suitable regularized version of the input random field is the key element of this method; we propose to regularize the random field by convolving the log-permeability with a Gaussian kernel. We analyze the mean square error of the estimator and the overall complexity of the algorithm. We also propose possible choices of the regularization parameter and of the number of samples per grid so as to equilibrate the space discretization error, the statistical error and the error in the computation of the expected value of the control variate by Stochastic Collocation. Numerical examples demonstrate the effectiveness of the method. A comparison with the standard Multi Level Monte Carlo method is also presented for different choices of the covariance function of the input field.

Approximation of Stratonovich SDEs and Travelling Waves.

Efthalia Tzitzili & Gabriel Lord *(Heriot-Watt University)*

In this talk, i present a new numerical method for approximating Stratonovich SDEs and give a strong convergence result. We then apply this to approximate travelling wave solutions and estimate the wave speed for stochastically forced PDEs. The wave position and hence the speed, is found by minimizing the L^2 distance between a reference function and the travelling wave.

Multilevel Estimation of Rare Events

Elisabeth Ullmann *(University of Bath)*

Estimation of failure probabilities is a fundamental problem in reliability analysis and risk management of engineering systems with uncertain inputs. We focus on systems described by partial differential equations (PDEs) with random coefficients. Failure events occur if some output process exceeds a given threshold. Monte Carlo simulation methods estimate the probability of failure events by sampling the random inputs and solving the associated PDE to obtain samples of the output process. However, in modern applications with highly resolved physical models and a possibly high-dimensional sample space the cost to obtain only a single output sample is nontrivial. If a large number of samples is required then the total computational cost might become prohibitively high.

Estimation of small failure probabilities associated with rare events poses serious computational challenges. The number of Monte Carlo samples required to achieve a given tolerance is inversely proportional to the probability of the rare event and can thus be too large for a given computational budget. The engineering community uses a more sophisticated Monte Carlo technique called Subset Simulation [Au & Beck, Prob. Eng. Mech., 2001] which is essentially a splitting algorithm applied to static problems. Subset Simulation reduces the total number of samples by decomposition of the sample space into a sequence of nested, partial failure sets. However, the physical discretisation of the engineering system – typically done by finite elements – is fixed in each failure set and sampling is still computing intensive as each sample requires the solution of a discretised PDE.

Minisymposium M7

Scalable Solvers for Large-Scale Partial Differential Equations

Organisers: Sébastien Loisel, Waad Subber and Hieu Nguyen

The 2-Lagrange Multiplier Method Applied to Nonlinear Transmission Problems for the Richards Equation in Heterogeneous Soil with Cross Points

Heiko Berninger & Sébastien Loisel & Oliver Sander *(Université de Genève)*

The Richards equation is a doubly nonlinear degenerate elliptic-parabolic partial differential equation used for the simulation of saturated-unsaturated groundwater flow. We formulate the 2-Lagrange multiplier method for the Richards equation in heterogeneous soil. This allows a rigorous formulation of a discrete version of the Richards equation on subdomain decompositions involving cross points. Using Kirchhoff

transformation, the individual subdomain problems in homogeneous soil can be transformed to convex minimization problems and solved efficiently using a monotone multigrid method. We discuss and compare weak formulations of the time-discrete and fully discretized multi-domain problem. It can be shown that in the case of two subdomains, when solving the resulting discrete system with a Richardson iteration, the new method is equivalent to a parallel nonlinear Robin method applied to the Richards equation. We give numerical results for a problem with realistic soil parameters.

Optimized Schwarz Methods for curl-curl time-harmonic Maxwell's equations

Victorita Dolean, Martin J. Gander, & Jin-Fa Lee & Zhen Peng *(University of Nice-Sophia Antipolis)*

Like the Helmholtz equation, the high frequency time-harmonic Maxwell's equations are difficult to solve by classical iterative methods. Domain decomposition methods are currently most promising: following the first provably convergent method in [2], various optimized Schwarz methods were developed over the last decade[5, 6, 1, 3, 7, 8, 4]. There are however two basic formulations for Maxwell's equation: the first order formulation, for which complete optimized results are known [3], and the second order, or curl-curl formulation, with partial optimization results [1, 7]. We show in this work that the convergence factors and the optimization process for the two formulations are the same. We then show by numerical experiments that the Fourier analysis predicts very well the behavior of the algorithms for a Yee scheme discretization, which corresponds to Nedelec edge elements on a tensor product mesh, in the curl-curl formulation. When using however mixed type Nedelec elements on an irregular tetrahedral mesh, numerical experiments indicate that transverse magnetic (TM) modes are less well resolved for high frequencies than transverse electric (TE) modes, and a heuristic can then be used to compensate for this in the optimization.

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Rational Krylov methods for transient electromagnetic geophysical forward modeling

Stefan Güttel *(The University of Manchester)*

Initial value problems for the quasi-static Maxwell's equations arising in transient electromagnetic modeling (TEM) can be solved efficiently in frequency or time domain via rational Krylov methods, provided that an efficient linear system solver is available. In this talk we will concentrate on the time domain problem, in which case $\exp(tA)v$, the action of the exponential of a large sparse symmetric matrix A onto a vector of initial values v, needs to be computed. Rational Krylov methods require sophisticated parameter selection strategies for achieving fast convergence. We will compare several parameter selection strategies proposed in the recent literature. We will also present a new simple parameter selection strategy that will give mesh independent convergence with a guaranteed error bound for a wide (but finite) range of time parameters $t \in [t_{\min}, t_{\max}]$.

This is joint work with Oliver G. Ernst (Chemnitz) and Ralph-Uwe Börner (Freiberg).

Solving Large systems using the 2-Lagrange multiplier methods

Anastasios Karangelis *(Heriot-Watt University)*

The 2-Lagrange multiplier method is a domain decomposition method based on solving Robin problems on the subdomains. I will discuss the parallel implementation of this method with cross points and present numerical experiments on Hector supercomputer. Moreover some recent improvements on the implementation will be presented.

Coarse grid correction for the Neumann–Neumann waveform relaxation method

Felix Kwok *(University of Geneva)*

The Neumann–Neumann waveform relaxation (NNWR) method has been proposed recently by Gander, Kwok and Mandal for the solution of parabolic problems, such as the heat equation. Just like for the steady case, one step of the method consists of solving the subdomain problems using Dirichlet traces, followed by a correction step involving Neumann interface conditions. However, each subdomain problem is now in both space and time, and the interface data to be exchanged are also functions of time. This method has been shown to converge superlinearly for finite time windows; however, as the number of subdomains increases, the required number of iterations for convergence to a fixed tolerance increases proportionally. We show that by adding a coarse grid correction step, the modified method converges in two iterations for 1D problems, independent of the number of subdomains. We also analyze its convergence rate for the 2D case.

This is joint work with Martin J. Gander (Geneva), Sébastien Loisel (Heriot-Watt), Bankim C. Mandal (Geneva) and Kévin Santugini (Bordeaux).

Efficient algorithms for large-scale problems

Sébastian Loisel *(Heriot-Watt University)*

In mathematics, physics, engineering, finance and other fields of science, boundary value problems play an important role. In many cases, the solution cannot be found in closed form and instead one must use a numerical approximation. In order to obtain an accurate approximation, one uses many grid points and thus one must solve a very large problem, requiring a very large parallel computer. It is surprisingly difficult to write a parallel program that outperforms a sequential program. In this talk, we will discuss some useful approaches to this challenging problem.

Fuzzy Domain Decomposition: a new perspective on heterogeneous DD methods

Jérôme Michaud *(University of Geneva)*

In a wide variety of physical problems, the complexity of the physics involved is such that it is necessary to develop approximations, because the complete physical model is simply too costly. One can then use heterogeneous domain decomposition techniques. But sometimes, information about the domain of validity of the available approximation are missing or incomplete or at least not a priori known.

In this talk we will introduce a new formalism for heterogeneous DD methods based on *Fuzzy Sets Theory* introduced by Zadeh in 1965. The idea is to fuzzy the boundary of the validity domain to obtain a smooth transition between the different approximations.

We will illustrate how the method works with some simple model problems and show some approximation quality results.

An Efficient Preconditioner for Parallel Adaptive Finite Element

Hieu Nguyen & Sébastian Loisel *(Heriot-Watt University)*

In parallel computing, it is advantageous to have data distributed across processors. However, one need to have mesh data structure of the whole domain to fully perform adaptive feedback loops in adaptive finite element. A solution for this dilemma is to use heterogeneous local meshes. These are meshes of the whole domain. They are fine in the subdomains they are associated with, but much coarser elsewhere. In this talk, we present a Schwarz-type preconditioner formulated based on these heterogeneous meshes. We prove that the convergence rate of the CG method, when paired with this preconditioner, depends only on the ratio of the second largest eigenvalue and the smallest eigenvalue. In addition, we can respectively bound these eigenvalues from above and below. The bounds depend on the minimum number of colours required to colour the subdomains in such a way that no neighbour are the same colour. However, they are independent of the mesh sizes. Numerical results will be provided to support our theoretical results.

Domain Decomposition Preconditioners for the Spectral Stochastic Finite Element Method

Waad Subber & Abhijit Sarkar *(Heriot-Watt University)*

The Spectral Stochastic Finite Element Method (SSFEM) is a popular computational tool for uncertainty quantification in many physical and engineering models. For large-scale models however, the SSFEM may become computationally challenging as the size of the resulting linear system grows rapidly with the mesh resolution and the order of the stochastic dimension. To effectively exploit high performance computing platforms, two-level domain decomposition preconditioners are proposed to efficiently quantify uncertainty in large-scale computational models in the framework of the SSFEM. In particular, primal-primal and dual-primal iterative substructuring techniques are described

for the solution of the SSFEM linear system. In the primal-primal approach, the continuity of the solution field is strictly enforced on a selected set of the interface nodes. For the remaining interface nodes, the continuity condition is weakly satisfied in an average sense. In the dual-primal approach, the continuity condition on the corner nodes is strictly satisfied and Lagrange multipliers are utilized to weakly enforce the continuity on the remaining interface nodes. These approaches provide a global mechanism to exchange information across the subdomains leading to scalable algorithms. For the numerical illustrations, two- and three-dimensional elliptic problems with spatially varying non-Gaussian coefficients are considered. The parallel performance of the algorithms are investigated with respect to the mesh size, subdomain size, fixed problem size per subdomain, order of stochastic expansion and level of uncertainty in the system parameters. The numerical experiments are performed on a Linux cluster using MPI and PETSc parallel libraries.

Minisymposium M8

Mathematics for Data Assimilation
Organisers
Igor Gejadze and Melina Freitag

Efficient Computation of the Posterior Covariance Matrix in Large-Scale Variational Data Assimilation Problems

Kirsty Brown *(University of Strathclyde)*

For a large-scale variational data assimilation problem, the PCM provides important information, for example, confidence intervals for the optimal solution. However, due to long computational times and memory limitations, it is not possible to assemble, store or manipulate the PCM explicitly at the finest representation level. One approach is to approximate the PCM by the inverse Hessian of the auxiliary control problem based on the tangent linear model constraints. The limited-memory representation of the inverse Hessian can be built on the basis of a small number (as compared to the state-vector dimension) of 'leading' Ritz pairs of the projected (preconditioned) Hessian computed by the Lanczos method. Clearly, the success of this approach depends on the quality of preconditioning applied.

For first-level preconditioning, the square root of the background covariance matrix is commonly used. However, if the sensor information impact on the optimal solution is significant, this is not sufficient and additional preconditioning is required. In this talk, we will discuss using a multilevel approach as a second-level preconditioner to reduce both computational costs and memory requirements. We anticipate that, using this approach, the memory needed to store the PCM will be reduced by at least an order of magnitude compared with a single level implementation, with similar or reduced computational cost in terms of flops.

A simple method for using a complex model within a particle filter

Phil Browne *(University of Reading)*

The problem of including a model within an ensemble data assimilation system is known to be non-trivial to all those who have implemented them. We approach this problem from the viewpoint of climatological DA, in which the models used are many millions of lines of codes, split into multiple programs and executables. As a result of decades of man-years of development, these codes do not lend themselves easily to being converted into a single subroutine with a predefined I/O type. This talk will show a very simple method of coupling a complex model to a data assimilation program, using MPI to communicate between separate executable codes.

As an example of the MPI coupling, the Lorenz 63 model will be coupled to the equivalent weights particle filter. In the under-observed case where only the z component of the state vector is observed, the need for this fully non-linear data assimilation scheme will be shown, as bimodal pdfs are reconstructed for the distribution of the unobserved variables x and y.

Sensitivity Analysis in Variational Data Assimilation

François-Xavier Le Dimet & Tran Thu Ha *(Université de Grenoble)*

A sensitivity analysis is defined by some response function and the variable with respect to which the sensitivity is evaluated. In many cases the observations have errors and it is important to estimate the impact of this error, if the state of the system is retrieved through a variational data assimilation then the observation is found only in the Optimality System (O.S.) . Therefore the sensitivity analysis has to be carried out on the optimality system, in that sense sensitivity analysis is a second order property and the O.S. can be considered as a generalized model because it contains all the available information. In this presentation we will see how a sensitivity analysis can be carried out.

The method is applied to water pollution. The model is derived from shallow waters equations and an equa-

tion of concentration of the pollutant, it is discretized using a finite volume method and the sensitivity with respect to the source term of the pollutant is studied.

Data assimilation as an inverse problem: theory and computational challenges

Melina A Freitag *(University of Bath)*

In this talk we aim to provide a theoretical framework for data assimilation, a specific type of an inverse problem arising for example in numerical weather prediction, hydrology and geology. We consider the general mathematical theory for inverse problems and regularisation, before introducing Tikhonov regularisation as one of the most popular methods for solving inverse problems. We show that data assimilation techniques such as 3DVar and 4DVar as well as the Kalman filter and Bayes' data assimilation are, in the linear case, a form of cycled Tikhonov regularisation. We give an introduction to key data assimilation methods as currently used in practice, provide an error analysis for the data assimilation process in general and explain computational challenges.

On practical observability of nonlinear dynamical systems in the variational data assimilation framework

Igor Gejadze *(University of Strathclyde)*

Problems of variational data assimilation are formulated as optimal control problems for a model governed by nonlinear PDEs with the goal of identifying the initial condition, boundary conditions or distributed parameters of the model. The input data contains the background, observation and model errors, hence the error in the optimal solution. This error is usually characterized by the analysis covariance matrix, which can be approximated by the inverse Hessian of the auxiliary cost function. Two errors in this covariance estimate (due to the nonlinearity) are considered: linearization error and origin error. For reducing the linearization error, a method based on computation of an ensemble of inverse Hessians is suggested (the Effective Inverse Hessian method). The origin error, however, cannot be reduced or eliminated by any algorithmic tool. As such, it limits our ability to verify the optimal solution, thus limiting observability of the system. A test for accessing a possible magnitude of the origin error is presented. This test reveals which parts of the estimated state vector cannot be verified. This information may be vital in several aspects of data assimilation, such as the ensemble generation for forecasting and design of adaptive observations. Numerical examples computed for the 1D Burgers' equation are presented throughout.

The Effects of Numerical Model Error in Data Assimilation

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

4D-Variational data assimilation (4D-Var) is typically used for forecasting physical systems. It finds an initial condition for a numerical model, by combining observations with predictions. The numerical model is then used to produce a forecast. Numerical model error affects the accuracy of the initial condition and its forecast.

Here the linear advection equation is chosen as the physical system, $u : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$,

$$u_t(x,t) + \eta u_x(x,t) = 0,$$

$\eta \in \mathbb{R}$. This system can be solved using a finite difference scheme, introducing numerical model error through the approximation of derivatives. The effect of this error on the initial condition found through 4D-Var is analysed in terms of numerical dissipation and dispersion. Here the Upwind, Preissman Box and Lax-Wendroff schemes are investigated.

Initially the effects of numerical model error on the initial condition are investigated in the absence of all other errors. Subsequently, observation errors are reintroduced into the problem. We find an upper bound for the l_2-norm of the error introduced into the initial condition in both cases. The order of convergence of the error to zero, with respect to both the number of discretisation points in space and the number of observations in the assimilation window is analysed.

Instability and regularization in data assimilation

A.S. Lawless & A.J.F. Moodey, R.W.E. Potthast, P.J. van Leeuwen *(University of Reading)*

Data assimilation is the process of incorporating observational data into a numerical model in order to estimate the state of a dynamical system. It forms an essential part of modern environmental forecasting systems, such as those used for weather and ocean prediction. At regular intervals the latest forecast from the numerical model is updated using new observations to provide an improved estimate of the current state, known as the *analysis* in data assimilation terminology. In many cases the operator that maps from state space to observation space leads to an ill-posed equation and stability of the inversion problem at each assimilation time is guaranteed by a form of Tikhonov regularization, using the forecast of the previous analysis as a prior estimate of the state. Several common data assimilation algorithms, including variational methods and Kalman filters, can be considered

in this framework.

In this work we examine the stability of the error in a sequence of analyses as the assimilation process is cycled in time. Since the data assimilation problem is often solved in very high dimensional systems (of order 10^8 and higher), we derive theory using an infinite-dimensional framework. We show that for linear model dynamics described by a Hilbert-Schmidt operator it is possible to guarantee the stability of the analysis error in time by choosing the regularization parameter sufficiently small. In the case of time-varying dynamics the regularization parameter can be chosen adaptively to ensure stability. However, as the size of the regularization parameter is reduced, the assimilation problem at each time is less well-conditioned and the bound on the analysis error increases. For nonlinear dynamics similar stability results are obtained under certain Lipschitz continuity and dissapitivity assumptions on the dynamical operator. The theory is illustrated with numerical results.

Nonlinear data-assimilation in high dimensions: Merging probabilistic and optimisation techniques

Peter Jan van Leeuwen *(University of Reading)*

The data-assimilation problem is most naturally formulated using Bayes theorem. This theorem states that prior information of the system under study is updated with observations by multiplying the prior probability density function (pdf) value of a model state with the likelihood of that model state given the observations to find the posterior pdf value of that model state, for each possible model state. This full posterior pdf is the solution to the data-assimilation problem, and as such this problem is a multiplication problem, and not an inverse problem. Although this formalism is completely general it is not easy to apply in general when the dimension of the system is large.

The data-assimilation problem becomes an inverse problem (in the sense that one has to solve a set of coupled (non-)linear equations) when one concentrates on the most probable model state of the posterior pdf. The state with maximum posterior pdf value is the same as the one that minimizes minus the log of this posterior pdf, and efficient iterative methods have been derived to find these minima, even for very high dimensional problems with up to a billion variables. It is well recognized that uncertainty information on this most probable state is needed to make this is a scientifically sound approach. If the posterior pdf is different from a Gaussian, for instance much broader, or even multi-modal, this information is not easily obtained using inverse methods.

A way forward is to use particle filters to solve Bayes theorem. The standard particle filter is degenerate when the number of independent observations is large, mainly because it is highly unlikely to end up close to al these observations. However, particle filters can be made efficient when a proper proposal (or importance) density is used, which in practice means that the particles are informed about future observations. This is where the connection with inverse methods becomes apparent: Inverse methods can be used on each particle to give them high likelihood, hence to make them efficient.

Simple implementations of inverse methods on individual particles have let to astonishingly good results. We will show applications of particle filters to systems with tens of thousands of independent observations, with formulations that theoretically have no limit on the number of independent observations. However, there are huge improvements possible when more sophisticated inverse methods are employed. Interestingly, the inverse problem changes from finding the best initial condition given the observations to finding the best model trajectory given the observations and given the initial condition, and that on each particle. An initial discussion on how to do this will be presented, hoping for a lively discussion on the way forward.

Analysis error covariance and posterior covariance in variational data assimilation

Victor Shutyaev & Igor Gejadze, Francois-Xavier Le Dimet *(Russian Academy of Sciences)*

The problem of variational data assimilation for a nonlinear evolution model is stated as an optimal control problem to estimate the analysis (initial condition) [1]. The data contain errors (observation and background errors), hence there is an error in the analysis. For mildly nonlinear dynamics, the analysis error covariance can be approximated by the inverse Hessian of the cost functional in the auxiliary data assimilation problem [2], whereas for stronger nonlinearity the 'effective' inverse Hessian approach may be used [3, 4]. However, the analysis error covariance is not the posterior covariance from the Bayesian perspective. While these two are equivalent in the linear case, the difference may become significant for nonlinear problems [5]. For the proper Bayesian posterior covariance a new approximation via the Hessian of the original cost functional is derived and its 'effective' counterpart is introduced. An approach for computing the analysis error covariance and posterior covariance in the matrix-free environment using Lanczos method with preconditioning is suggested. Numerical exam-

ples which validate the developed theory are presented for the model governed by the Burgers equation with a nonlinear viscous term.

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Minisymposium M9

Mathematics and Algorithms Related to Chebfun

Organiser: Nick Hale

The linear barycentric rational quadrature method for Volterra integral equations

Jean–Paul Berrut *(University of Fribourg)*

We shall first introduce linear barycentric rational interpolation to the unaware audience : it can be viewed as a small modification of the classical interpolating polynomial. Then we present two direct quadrature methods based on linear rational interpolation for solving general Volterra integral equations of the second kind. The first, deduced by a direct application of linear barycentric rational quadrature given in former work, is shown to converge at the same rate, but is costly on long integration intervals. The second, based on a composite version of the rational quadrature rule, looses one order of convergence, but is much cheaper. Both require only a sample of the involved functions at equispaced nodes and yield a stable, infinitely smooth solution of most classical examples with machine precision.

Computing multiple solutions of nonlinear ODEs with Chebfun

Asgeir Birkisson *(University of Oxford)*

In this talk, we will review the capabilities Chebfun offers for finding multiple solutions of nonlinear boundary-value problems of ordinary differential equations. Chebfun offers two methods for obtaining such multiple solutions; one is path-following in infinite dimensions, and the other is deflation of solutions for differential operators. Both approaches will be described, and examples given of their use.

Fast Chebyshev to Jacobi transforms using asymptotic expansions

Nick Hale & Alex Townsend *(University of Oxford)*

In this talk we describe a simple algorithm for transforming between function values $\{f_j\}_{j=0}^N$ of a degree N polynomial $f(x)$ evaluated on an $(N+1)$-point Chebyshev grid and the coefficients of any of its Jacobi polynomial expansions

$$f(x) = \sum_{n=0}^{N} c_n^{\alpha,\beta} P_n^{(\alpha,\beta)}(x), \qquad \alpha, \beta > -1.$$

In the special case $\alpha = \beta = 0$ this gives a *fast Legendre transform* from a Chebysghev grid to Legendre coefficients (and vice versa). The algorithm is based upon asymptotic expansions derived by Steiltjes and Hahn for $P_n(x)$ and $P_n^{(\alpha,\beta)}(x)$ of large degree which can be expressed in a form amenable to evaluation via a fast Fourier transform (FFT).

Rational integration of analytic functions from equispaced data

Georges Klein & Stefan Güttel *(University of Oxford)*

Linear barycentric rational interpolation from equispaced data does not lead to the Runge phenomenon and is well-conditioned. Moreover, if the interpolated function is analytic, high-order approximation can be achieved. We show that this also holds true for the approximation of antiderivatives and present some applications using Chebfun.

An extension of Shepard interpolation with quadratic approximation order

Filomena Di Tommaso & Francesco Dell'Accio & Kai Hormann *(Universit della Calabria)*

Shepard's method [2] is a well-known technique for interpolating large sets of scattered data. The classical Shepard operator reconstructs an unknown function as a normalized blend of the function values at the scattered points, using the inverse distances to the scattered points as weight functions. In this talk we extend the bivariate Shepard operator in two ways. On the one hand, we consider a triangulation of the scattered points and substitute function values by linear polynomials which locally interpolate the given data at the vertices of each triangle [1]; here the usual restriction that each triangle side is entirely shared by two adjacent triangles is not necessarily required. On the other hand, we modify the classical point-based weight functions and define instead a normalized blend of the locally interpolating polynomials with triangle-based weight functions which depend on the product of inverse distances to the three vertices of the corresponding triangle. The resulting operator interpolates all data required for its definition and reproduces polynomials up to degree 1, whereas the classical Shepard operator reproduces only constants. As a consequence, this interpolation operator has quadratic approximation order, which is confirmed by our numerical results.

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Chebfun2: An extension of Chebfun to two dimensions

Alex Townsend & Nick Trefethen *(Oxford University)*

An object-oriented MATLAB system is described that extends the capabilities of Chebfun to smooth functions of two variables defined on rectangles. Functions are approximated to essentially machine precision by using iterative Gaussian elimination with complete pivoting to form "chebfun2" objects representing low rank approximations. Operations such as integration, differentiation, function evaluation, and transforms on chebfun2 objects can be particularly efficient. Furthermore, global optimization, the singular value decomposition, and rootfinding are also performed on chebfun2 objects with some interesting algorithms.

What would "Diskfun" look like?

Lloyd N. Trefethen *(University of Oxford)*

Although real intervals are the most basic domains for applications, the complex unit disk is the more fundamental domain mathematically. Most of the theorems and algorithms of approximation theory that Chebfun is built on have simpler analogues on the disk. We review this subject.

Computing Complex Singularities of Differential Equations with Chebfun

Marcus Webb *(University of Cambridge)*

Given a solution to an ordinary differential equation on a time interval, the solution for complex-valued time may be of interest, in particular whether the solution is singular at some complex time value. How can the solution be approximated in the complex plane using only the data on the interval? A polynomial approximation of the solution always fails to capture singularities; to extrapolate solutions with singularities, approximation with rational functions is more appropriate. However, most rational approximation methods have the issue that spurious poles appear for all but the simplest functions, even in exact arithmetic. We discuss and demonstrate Chebfun's implementation of a *robust* rational interpolation and least squares algorithm based on the work of Pachón, Gonnet, Van Deun and Trefethen, ideal for the aforementioned problem. Examples include Lorenz and Lotka–Volterra equations.

Computing Inverse Functions

Kuan Xu *(Oxford University)*

In this talk, we will first review the existing algorithm for computing a general inverse function and the limitation of the current Chebfun implementation. A new but very simple algorithm will be presented. Breaking points are introduced to partition the domain of the inverse functions and in each of these sub-domains the inverse function is approximated by a piecewise smooth chebfun. This 'splitting-on' functionality significantly speeds up the computation and broadens the applicability of the Chebfun 'inverse' function. A few numerical examples will be discussed to show the efficiency of the proposed algorithm.

Minisymposium M10

Developments in Preconditioners and Iterative Methods for Linear Systems
Organisers
Jennifer Pestana and Eric de Sturler

Recycling Preconditioners for Sequences of Systems

Eric de Sturler *(Virginia Tech)*

We will discuss efficient methods and underlying theory for updating preconditioners for a range of applications, such model reduction, inverse problems, quantum Monte Carlo methods, and acoustics.

How DG Discretizations Influence the Convergence of Block Jacobi Preconditioning

Soheil Hajian & Martin J. Gander *(Université de Genève)*

A block Jacobi method can be viewed as an iterative method applied to a preconditioned system. For classical discretizations of elliptic partial differential equations, like conforming finite element methods (FEM) or finite difference methods (FDM), block Jacobi iterations are equivalent to classical Schwarz iterations with Dirichlet transmission conditions. This is however not necessarily the case for discontinuous Galerkin methods (DG). We will show in this talk for the model problem $(\eta - \Delta)u = f$ and various DG discretizations that a block Jacobi method applied to the discretized problem can be interpreted as a Schwarz method with different transmission conditions from the classical Dirichlet ones.

The convergence of the block Jacobi method of these DG methods depends directly on the penalty parameter of the DG method. The results from non-overlapping Schwarz methods suggest that the usual choice for this parameter will result in very slow convergence of block Jacobi iterations. We then show how to modify the scheme in order to obtain fast convergence of the corresponding block Jacobi methods while preserving the approximation properties of the DG method.

On some preconditioning techniques for incompressible Navier-Stokes equations

Xin He & Kees Vuik *(Delft University of Technology)*

The focus of this work is on fast and reliable preconditioning techniques for solving the incompressible Navier-Stokes equations, which consist of a set of coupled nonlinear partial differential equations.

In general, after linearization and finite element discretization in space, the original nonlinear problem is converted into finding the solutions of a sequence of linear systems of equations. Because of the underlying mathematical model, the coefficient matrix of the linear system is indefinite and nonsymmetric of two-by-two block structure. Due to their less demands for computer resources than direct methods, iterative solution methods are chosen to solve these linear systems. In order to accelerate the convergence rate of the iterative methods, efficient preconditioning techniques become essential. Fast and reliable preconditioners for the matrices arising from Navier-Stokes equations with constant density and viscosity have been studied intensively during the past decades, see the survey paper [1] and the references therein, and is also a main concern in this work. We contribute to the search of efficient preconditioners by thoroughly analyzing and testing the so-called augmented Lagrangian method [2]. The comparison between the augmented Lagrangian preconditioner and other well-known preconditioners, e.g., the SIMPLER-type preconditioner [4], is also illustrated.

The Navier-Stokes equations with constant density but variable viscosity may arise in multiphase flow problems. In the mixture system, the problem parameters, such as density and viscosity, remain constant within each phase due to the assumption that each phase flow is immiscible and incompressible. However, they vary sharply and smoothly across the interfaces, that evolve with time and space. An illustrative example for such a system is a mixture of water and oil, which have the same density, however their viscosities differ much. Variable viscosity has its impact on the behavior of preconditioners, shown to be efficient for the constant viscosity case. Those preconditioners have to be reconsidered and analyzed in order to show their robustness with respect to varying viscosity. In this work we choose the augmented Lagrangian method, and not only numerically but also theoretically show that the corresponding preconditioner preserves its high quality also for spatially varying viscosity.

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Hierarchical preconditioners for higher-order FEM

Sabine Le Borne *(Technische Universität Hamburg-Harburg)*

The finite element discretization of a partial differential equation requires the selection of a suitable finite element space. While higher order finite elements (HOFEMs) lead to finite element solutions of higher accuracy, their associated discrete linear systems of equations are often more difficult to solve than those of lower order elements.

In this talk, we present efficient preconditioners for the solution of linear systems of equations associated with HOFEMs. More sprecifically, we will use the technique of hierarchical ($\mathcal{H}$-) matrices for the construction of $\mathcal{H}$-LU preconditioners for these HOFEM stiffness matrices. $\mathcal{H}$-matrices provide a powerful technique to compute and store approximations to dense matrices in a data-sparse format. The basic idea is the approximation of matrix data in hierarchically structured subblocks by low rank representations. We will distinguish between blackbox $\mathcal{H}$-LU preconditioners which factor the entire stiffness matrix and hybrid methods which use $\mathcal{H}$-LU factorization only for certain subblocks of the matrix.

We illustrate all introduced preconditioners with supporting numerical results.

Fast Iterative Solution of PDE-Constrained Optimization Problems

John W. Pearson *(University of Oxford)*

In this talk, we discuss the numerical solution of PDE-constrained optimization problems, an important class of problems within numerical analysis and applied science. In particular, we seek to develop preconditioned iterative solvers for the matrix systems arising from a number of such problems.

The general approach we employ is to examine the systems involved, which are of saddle point structure, and construct effective approximations of the $(1,1)$-block and Schur complement of the matrices. We then apply these approximations within iterative methods such as MINRES, non-standard Conjugate Gradients and GMRES.

We find that this strategy is a viable one for a wide range of PDE-constrained optimization problems. In this talk, we first examine simpler problems such as Poisson control, and then extend our methodology to PDE-constrained optimization problems arising from fluid dynamics, as well as time-dependent problems. In each case, we motivate the preconditioners selected, state eigenvalue bounds of the preconditioned systems where relevant, and display numerical results to highlight the performance of our solvers in practice.

GMRES convergence bounds that depend on the right-hand side vector

Jennifer Pestana & David Titley-Peloquin & Andrew Wathen *(University of Oxford)*

GMRES is one of the most popular matrix-free iterative methods for solving linear systems $Bx = b$ where $B \in \mathbb{C}^{n\times n}$ and $b \in \mathbb{C}^n$. This makes the description of its convergence an important topic of investigation. Many convergence bounds start from the ideal GMRES problem. In contrast, in this talk we present bounds for linear systems with nonsingular, diagonalizable coefficient matrices that explicitly include the right-hand side vector. We show that the GMRES residual norm satisfies a weighted polynomial least-squares problem on the spectrum of B, and that GMRES convergence reduces to an ideal GMRES problem on a rank-one modification of the diagonal matrix of eigenvalues of B. Numerical experiments show that these bounds can accurately describe the convergence of GMRES.

Block Diagonal Preconditioners for Optimization Problems

Tyrone Rees *(STFC Rutherford Appleton Laboratory)*

One of the major bottlenecks in modern optimization codes is the requirement to solve multiple so-called saddle point systems of the form

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

For example, primal-dual interior point methods apply variants of Newton's method to a non-linear system to find a minimum of constrained quadratic program. This method requires the solution of a sequence of saddle point systems of the form above – called the augmented system in this context – at each step of the Newton iteration.

In many situations – especially for large scale optimization problems – we would like to solve the saddle point system iteratively, as computing the factorizations at each Newton step to employ a direct solver

would be prohibitively expensive. However, it is important to choose the iterative solver so that the errors are sympathetic to the outer Newton iteration. For this reason Krylov subspace methods with constraint preconditioners, i.e., preconditioners of the form

$$P_{con} = \begin{pmatrix} G & B^T \\ B & 0 \end{pmatrix},$$

have been popular in the optimization community, as they are known to preserve the constraints, and this fact can be used to prove convergence of the inexact Newton method. However, applying such a preconditioner can be costly, and ensuring that the solution remains on the constraint manifold in the presence of rounding errors can be delicate.

Block diagonal preconditioners of the form

$$P_{bd} = \begin{pmatrix} A & 0 \\ 0 & S \end{pmatrix}$$

have proved successful in, e.g., the field of computational fluid dynamics, due to their ease of application and effectiveness. However, giving conditions for the convergence of an inexact Newton method when using such an iterative method is not trivial.

In this talk I will describe a way to combine both of these preconditioners in an inner iteration, using the easy to apply block diagonal preconditioner to do most of the work, and then using one application of the constraint preconditioners to project the approximate solution onto the constraint manifold. We hope that this will increase the number of types of preconditioners which can be used safely in constrained optimization problems, and therefore will lead to the development of more high-quality preconditioners tailored to this important field.

Solving Ill-posed Linear Systems with GMRES

Valeria Simoncini & Lars Eldén *(Università di Bologna)*

Almost singular linear systems arise in discrete ill-posed problems. Either because of the intrinsic structure of the problem or because of preconditioning, the spectrum of the coefficient matrix is often characterized by a sizable gap between a large group of numerically zero eigenvalues and the rest of the spectrum. Correspondingly, the right-hand side has leading eigencomponents associated with the eigenvalues away from zero. In this talk the effect of this setting in the convergence of the Generalized Minimal RESidual (GMRES) method is considered. It is shown that in the initial phase of the iterative algorithm, the residual components corresponding to the large eigenvalues are reduced in norm, and these can be monitored without extra computation. The analysis is supported by numerical experiments on singularly preconditioned ill-posed Cauchy problems for partial differential equations with variable coefficients.

Do Ritz values influence the convergence behavior of restarted GMRES?

Jurjen Duintjer Tebbens & Gérard Meurant *(Academy of Sciences of the Czech Republic)*

This talk is based on the work by Arioli, Greenbaum, Pták and Strakoš proving that any residual norm history is possible for full GMRES with any nonzero spectrum. We recently showed that this is in fact possible with any set of Ritz values for all iterations of the GMRES process. We will address the practically more relevant situation where GMRES is restarted and show that arbitrary convergence curves are not possible anymore. We will in particular show that prescribed residual norms in one restart cycle can predetermine the residual norms for the next cycle and we discuss the relation of this phenomenon with Ritz values and possible consequences for restarting with a deflation technique. We also address prescribing the Ritz values generated during the subsequent restart cycles.

Minisymposium M11

Adaptive Methods in Fluid Mechanics

Organiser: Malte Braack

Model- and mesh adaptivity for transient problems

Malte Braack & Nico Taschenberger *(Technische Universität Darmstadt)*

We propose a duality based a posteriori error estimator for the computation of functionals averaged in time for nonlinear time dependent problems. Such functionals are typically relevant for (quasi-)periodic solutions in time. Applications arise, e.g. in chemical reaction models. In order to reduce the numerical complexity, we use simultaneously locally refined meshes and adaptive (chemical) models. Hence, considerations of adjoint problems measuring the sensitivity of the functional output are needed. In contrast to the classical dual-weighted residual (DWR) method, we favor a fixed mesh and model strategy in time. Taking advantage of the (quasi-)periodic behaviour, only stationary dual problems have to be solved.

Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows

Jens Lang *(Technische Universität Darmstadt)*

Moving Meshes in Large Eddy Simulation for Turbulent Flows In the last years considerable progress has been made in the development of Large Eddy Simulation (LES) for turbulent flows. The characteristic length scale of the turbulent fluctuation varies substantially over the computational domain and has to be resolved by an appropriate numerical grid. We propose to adjust the grid size in an LES by adaptive moving meshes. The monitor function, which is the main ingredient of a moving mesh method, is determined with respect to a quantity of interest (QoI). These QoIs can be physically motivated, like vorticity, turbulent kinetic energy or enstrophy, as well as mathematically motivated, like solution gradient or some adjoint-based error estimator. The main advantage of mesh moving methods is that during the integration process the mesh topology is preserved and no new degrees of freedom are added and therefore the data structures are preserved as well. We will present results for real-life engineering and meteorological applications.

Residual-based adaptive turbulence modelling with quantitative a posteriori error control

Aurèlien Larcher & Johan Hoffman *(Royal Institute of Technology KTH)*

We present some elements of adaptive simulation of incompressible turbulent flows, and we focus in particular on residual-based turbulence modelling with a posteriori error control.

Turbulent flows are at the heart of a number of problems in science and engineering, such as computing aerodynamic forces around cars and airplanes. In realistic problems, full resolution of turbulent scales is not possible. Thus, development of accurate subgrid models based on the theory of fluid mechanics and experimental measurements, is a key challenge of LES. As an alternative to commonly used RANS and LES approaches stands the so-called Implicit LES (ILES), for which the construction of an explicit subgrid viscosity based on physical arguments is not required, but instead the subgrid model is contained in the discretization of the NavierStokes equations.

In the context of finite element approximations, we have developed an ILES method based on numerical stabilization of the NavierStokes equations in terms of the residual [3, 5], similarly to other approaches developed in the past few years with the intention to provide a mathematical framework to LES.

In [3, 5, 4] we have extended a framework for a posteriori error estimation to LES. The framework, described e.g. in [1, 6, 2], involves using the solution of an adjoint problem to obtain an a posteriori estimate of the error for a chosen output functional of the solution. With a residual-based subgrid model, ILES fits naturally into this framework: in this case the subgrid model represents a computable modelling error. We present the computational framework developed for the numerical simulation of turbulent flows on supercomputers and some validation examples used to evaluate the implemented method.

[1] K Eriksson, D. Estep, P. Hansbo, C. Johnson: Introduction to adaptive methods for differential equations. Acta Numer., 4 (1995), 105158.
[2] M. Giles and E. Süli: Adjoint methods for PDEs: a posteriori error analysis and postprocessing by duality. Acta Numer., 11 (2002), 145236.
[3] J. Hoffman, C. Johnson: A new approach to Computational Turbulence Modeling. Comput. Methods Appl. Mech. Engrg., 195 (2006), 28652880.
[4] J. Hoffman, Computation of mean drag for bluff body problems using Adaptive DNS/LES. SIAM J. Sci. Comput., 27 (2005), 184207.
[5] J. Hoffman, C. Johnson: Computational Turbulent Incompressible Flow. Applied Mathematics: Body and Soul, Volume 4. Springer, 2007.
[6] R. Becker, R. Rannacher: A posteriori error estimation in finite element methods. Acta Numer., 10 (2001)

Anisotropic error estimates and space adaptivity for a semi-discrete finite element approximation of the transient transport equation

Marco Picasso *(Technische Universität Darmstadt)*

A stabilized semi-discrete finite element discretization of the transient transport equation is studied in the framework of anisotropic meshes. A priori and a posteriori error estimates are derived, the involved constants being independent of the mesh aspect ratio, only space discretization being considered.

Numerical results on non adapted, anisotropic meshes and small time steps confirm the sharpness of the theoretical predictions. An anisotropic, adaptive finite element algorithm is then proposed with goal to control the L^2 error in space at final time, the time step being kept constant. Numerical results are then presented on anisotropic, adapted meshes and small time steps. Three different methods are proposed to interpolate the solution between two adapted meshes.

Minisymposium M12

Algorithms for Networks and Collective Behaviour
Organisers
Alastair Spence & Des Higham

Betweenness Centrality Measures for Dynamic Networks

Ahmad Alsayed *(University of Strathclyde)*

Many emerging network data sets are time dependent. In this talk, we propose new temporal and nodal betweenness measures for such dynamic networks. They are defined by extending the classical concept of betweenness in static networks to the case of transient edges. The new measures quantify which nodes and which time points are important in terms of network perturbation. We finish with examples showing the new two measures applied to real and synthetic data.

Developing an evolving network model based on an extension of the triadic closure concept

Erzsebet Dombi & Desmond J. Higham *(University of Strathclyde)*

A wide variety of networks appearing in real life applications are inherently dynamic, with edges forming and vanishing over time. It has been observed by social scientists that triangles tend to close in such networks—friends-of-friends tend to become friends. This concept has become known as the triadic closure principle. Based on this principle, a nonlinear network evolution model was introduced in [1] by Grindrod, Higham and Parsons and a mean field theory was developed, which predicted bistable behaviour in the long term. Computational results confirmed this prediction. The triadic closure concept can be extended if the likelihood of n-cycles forming ($n \geq 4$) at the next time step is also increased; for example, a new friendship is more likely to arise if there are many mutual friends-of-friends. We investigate whether a network evolution model with corresponding mean-field theory can be developed based on this extension of the triadic closure concept.

[1] P. Grindrod, D. Higham and M.C. Parsons, *Bistability through triadic closure,* Internet Mathematics 8 (4), 2012, pp.402-423.

Gone in 20 Minutes

Desmond J Higham *(University of Strathclyde)*

I will present volume-across-time data from several Twitter conversations. My interest is in the spikes of Twitter activity that can be attributed to high profile events or news items (for example, a red card in a Premier League soccer game). In each case, we observe that the initial spike decays with a recognisable half-life, typically of around 20 minutes. These dramatic, but short-lived, bursts of interest represent marketing opportunities for suitably agile players (as demonstrated by the cookie company Oreo in the 2013 Superbowl). To understand the nature of the spike-and-decay activity, we propose a discrete time model that takes account of the specific nature of Twitter communication: a fixed underlying tweeter-follower network forms the backbone of a dynamic message-passing process. Our model predicts that a certain network centrality measure plays a key role in describing the spread of information. We test this prediction on real Twitter decay data and then use the model to calibrate the rate at which news goes stale.

This is joint work with Fiona Ainley, Peter Grindrod, Peter Lalfin, Alex Mantzaris and Amanda Otley.

The How and Why of Balancing

Philip A. Knight *University of Strathclyde*

We consider the problem of taking a matrix A and finding diagonal matrices D and E such that the rows and columns of $B = DAE$ satisfy some specific constraints. Examples of constraints are that

- the row and column sums of B should all equal one;
- the norms of the rows and columns of B should all be equal;
- the row and column sums of B should take values specified by vectors p and q.

Simple iterative algorithms for solving these problems have been known for nearly a century. We provide a simple framework for describing these algorithms that allow us to develop robust convergence results and describe a straightforward approach to accelerate the rate of convergence.

Balancing has diverse applications from preconditioning to psephology. In this talk we focus on its use as a centrality measure.

Bridges in Twitter Networks

Alexander Mantzaris *(University of Strathclyde)*

Twitter has allowed the collection of very large scale

networks, giving fascinating snaphots of social interactions. Examples based on Twitter conversations from a diverse range of topics will be presented. There has been a substantial amount of work done on detecting communities from network connectivity data and some of the established methods will be described. When the community structure of a network is understood, we find that some of the nodes and edges play important bridging roles. I will focus on the discovery of these bridges, which are typically quite sparse in relation to the size of the communities. We will see that bridges are not always created by single edges, and there are many ways in which communities can be linked.

Perturbation Theory for Eigenvalues of Symmetric Matrices arising in Network Analysis

Alastair Spence *(University of Bath)*

Symmetric matrices, for example, the Laplacian and adjacency matrices, play an important role in the analysis of undirected networks. In particular, the eigenvectors corresponding to important eigenvalues are often used to produce low-dimensional representations of a network, as is the case with spectral clustering. In network applications edge weights are often subject to random perturbations and it is of interest to study how these perturbations affect the eigenvalues and eigenvectors of the associated matrices and, as a consequence, the associated low-dimensional representation of the network. In this talk we consider some perturbation theory for eigenvalues of symmetric matrices subject to random perurbations leading to the perturbed eigenvalues and eigenvectors being random variables. We shall look at how classical perturbation theory extends to the case of random perturbations.

This is joint work with Dr. Zhivko Stoyanov (University of Reading).

Minisymposium M13

Some Numerical Methods in Liquid Crystals

Organiser: Chuck Gartland

Some numerical aspects of liquid-crystal director modeling: motivation and Newton-like methods

Chuck Gartland & Alison Ramage *(Kent State University)*

Many continuum models for the orientational properties of liquid crystals involve one or more state variables that are vector fields of unit length. The pointwise unit-vector constraints associated with discretizations of such models give rise to indefinite linear systems of saddle-point form when these constraints are imposed via Lagrange multipliers. In problems such as these, indefiniteness also frequently manifests itself due to another influence (coupling with an applied electric field), and this leads to a *double* saddle-point structure. We are interested in the efficient numerical solution of large sparse linear systems associated with such problems.

These models are nonlinear and depend on multiple physical and geometric parameters, and it is typical for the equilibrium solutions (phases) to undergo transitions at critical values of certain of these parameters. The context we imagine is the numerical bifurcation and phase analysis of a discretization of a model for a realistic device or experiment. In such a setting, parameter continuation leads to the repeated solution of systems of the type we are studying. Good initial guesses are available, however, and global Newton methods are generally employed.

To motivate our work, we will present a realistic application, as well as a model, prototype problem, which embodies all of the essential features. In order to take greater advantage of the particular structure of these problems, we have developed a certain global Newton-like scheme, which we will discuss. The scheme retains the local quadratic convergence of the basic Newton Method but has some advantages.

An adaptive moving mesh method for a Q-tensor liquid crystal model

Craig MacDonald & John Mackenzie & Alison Ramage *(University of Strathclyde)*

In this talk we will describe a robust and efficient numerical scheme for solving the system of six coupled partial differential equations which arises when using **Q**-tensor theory to model the behaviour of a nematic liquid crystal cell under the influence of an applied electric field. Specifically, we consider a time-dependent problem in a Pi-cell geometry (which admits two topologically different equilibrium states) and model the order reconstruction which occurs. The adaptive non-uniform finite element mesh is generated by solving a moving mesh PDE based on the equidistribution of a strictly positive monitor function. We explore the use of three different monitor functions that are all based on a specific property of the **Q**-tensor and show that significant improvements in terms of solution accuracy and computational efficiency can be obtained using the correct choice of the monitor function. In addition, we use adaptive time-step control to ensure the accurate predicting of the

Some numerical aspects of liquid-crystal director modeling: stability and preconditioning

Alison Ramage & Chuck Gartland *(University of Strathclyde)*

In this presentation, which is a continuation of the previous talk (*Some numerical aspects of liquid-crystal director modeling: motivation and Newton-like methods* by Chuck Gartland), we investigate in more detail some properties of the indefinite linear systems of saddle-point form which arise from liquid-crystal director modeling. Specifically we show that, although the characterisation of local stability of solutions is complicated by the double saddle-point structure, efficiently computable criteria can be developed in terms of minimum eigenvalues of certain projected Schur complements. In addition, we discuss preconditioned iterative solvers for the individual linear systems which arise during a parameter continuation process. Both of these considerations are important when seeking a pracical method for computing phase diagrams.

Abstracts of Contributed Talks

Stability of space-time Petrov-Galerkin discretizations for parabolic evolution equations

Roman Andreev *(University of Maryland)*

In view of applications in e.g. optimal control problems with parabolic PDE constraints and massively parallel computations of time-dependent problems, space-time compressive discretizations of parabolic evolution equations are of increasing interest. In this talk we discuss space-time (sparse) tensor product simultaneous Petrov-Galerkin discretizations of parabolic evolution equations, and propose efficient preconditioners the iterative solution of the resulting single linear system of equations. Therein, space-time stability of the discretization, i.e., the validity of the discrete inf-sup condition with respect to suitable space-time norms uniformly in the discretization parameters, is essential. Viewing the Crank-Nicolson time-stepping scheme as a space-time Petrov-Galerkin discretization, we show that it is conditionally space-time stable. This motivates a general minimal residual Petrov-Galerkin discretization framework along with space-time stable families of trial and test spaces of (sparse) tensor product type, resulting in space-time compressive discretization algorithms.

Bernstein-Bézier Vector Finite Elements

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

Bernstein-Bézier techniques are known to be very effective for the computation with piecewise polynomials represented over a simplicial partition, which makes them an important tool in computationally demanding applications such as CAGD and visualisation, and in the finite element analysis relying on the discretization of the Sobolev spaces H^s. Here, we construct a basis for arbitrary order polynomial valued finite elements in the space $H(\mathrm{curl})$ using Bernstein-Bézier polynomials, and demonstrate the advantages of such an approach: Building upon sum factorization techniques which are available for the computation of the Bernstein-Bézier moments, our vector finite elements are the first to achieve optimal complexity on simplicial elements. The basis is useful for the solution of practical problems such as the numerical approximation of Maxwell's equations.

The Matrix Unwinding Function

Mary B. Aprahamian & Nicholas J. Higham *(University of Manchester)*

Multivalued functions f do not always satisfy the relation $f(f^{-1}(z)) = z$ for $z \in \mathbb{C}$. Motivated by this we consider multivalued matrix functions with arguments in $\mathbb{C}^{n\times n}$. In this talk we introduce the matrix unwinding function, $\mathcal{U}$, which describes the discrepancy between a matrix and the *principal* logarithm of its exponential,

$$\mathcal{U}(A) = \frac{A - \log \mathrm{e}^A}{2\pi i}.$$

We show that the unwinding function is instrumental in the derivation of correct identities involving logarithms and facilitates the understanding of other complex multivalued matrix functions, including inverse trigonometric functions.

We give a numerical scheme for computing the matrix unwinding function and show how it can be used to compute the matrix exponential using the idea of *argument reduction*. In general argument reduction methods for computing $f(A)$ consist of constructing a matrix C such that $f(C)$ and $f(A)$ are simply related and computing $f(C)$ is more favourable. Here we exploit the periodicity of the complex exponential function to compute $\mathrm{e}^A = \mathrm{e}^{\mathrm{mod}(A)}$, where $\mathrm{mod}(A) = A - 2\pi i\mathcal{U}(A)$. We show that applied in conjunction with the scaling and squaring algorithm, argument reduction can provide significant reductions in the cost of computations of the matrix exponential.

Projection-Based Methods for Eigenvalue Problems

Anthony P. Austin & Lloyd N. Trefethen *(University of Oxford)*

Let A be a large square matrix. How can we compute the eigenvalues of A that lie in a given region of the complex plane? A recent class of methods attacks this problem by "projecting" the matrix onto the region of interest, greatly reducing the problem's dimension. Perhaps the best known of these is the FEAST algorithm due to Polizzi, which may be applied to both standard and generalized Hermitian eigenvalue problems. In this talk, we will describe the principles underlying these methods. In particular, we shall explore modifications to the FEAST idea based on (a) the use of different rational functions as projection filters and (b) linearized rational interpolation.

Defect-based error estimates for exponential splitting methods

Winfried Auzinger & H. Hofstätter, O. Koch, and M. Thalhammer *(Vienna University of Technology)*

We consider exponential splitting methods for linear and nonlinear evolution equations of the form

$$\dot{u} = A(u) + B(u), \quad u(0) \text{ given.} \tag{7}$$

Splitting methods approximating the solution of (**??**) are based on separate integration of subproblems. E.g., the first-order Lie-Trotter method evaluates $\mathcal{S}(t,u) := \varphi_B(t, \varphi_A(t,u))$ in each integration step starting from u, with stepsize t. Higher-order methods are obtained by multiplicative recombination of several stages of this type, with appropriately chosen coefficients.

In [1-3], local error estimators are derived and analyzed. These are constructed in the form of quadrature approximations for an integral representation of the local error, involving evaluation of the defect

$$\mathcal{D}(t,u) = \dot{\mathcal{S}}(t,u) - A(\mathcal{S}(t,u)) - B(\mathcal{S}(t,u)) \tag{8}$$

of the splitting approximation $\mathcal{S}(t,u)$. Here, the derivative $\dot{\mathcal{S}}$ can be evaluated exploiting evolution equations satisfied by the stages constituting $\mathcal{S}$. These estimators can be shown to be asymptotically correct under appropriate regularity assumptions. In particular, evolution equations of Schrödinger type have been considered in detail.

In this talk we give an overview on to two major topics:

- Higher-order methods for linear problems: We sketch a new methodology for deriving a non-redundant set of order conditions via asymptotic expansion of the defect $\mathcal{D}(t) \cdot u$, involving iterated commutators of the operators A and B. This provides the basis for deriving a priori error estimates and proving asymptotic correctness of the defect-based error estimator.
- First- and second-order methods for nonlinear problems: We indicate how the defect-based approach can be extended to the nonlinear case. For the analysis, the local error is again expanded in terms of the defect $\mathcal{D}(t,u)$. Numerical evaluation of the defect is demonstrated for a cubic nonlinear Schrödinger equation.

We also present numerical results for exponential splitting combined with spectral discretization in space, applied to linear and nonlinear Schrödinger equations.

[1] W. Auzinger, O. Koch, M. Thalhammer, Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part I: The linear case, J. Comput. Appl. Math. 236 (2012) 2643–2659.
[2]W. Auzinger, O. Koch, M. Thalhammer, Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part II: Higher-order methods for linear problems, submitted to J. Comput. Appl. Math.
[3]W. Auzinger, H. Hofstätter, O. Koch, M. Thalhammer, Defect-based local error estimators for splitting methods, with application to Schrödinger equations, Part III: The nonlinear case, in preparation.

Model-based Sketching and Recovery with Expanders

Bubacarr Bah, Luca Baldassarre & Volkan Cevher *(EPFL)*

We study a traditional *linear sketching* and *compressed sensing* problem of obtaining an approximation of $\mathbf{x}$ from its noisy sketch (measurement) $\mathbf{Ax} + \mathbf{e}$ by leveraging prior knowledge about $\mathbf{x}$, where $\mathbf{A}$ is a sketching (measurement) matrix and $\mathbf{e}$ is a bounded perturbation term. In this setting, standard approaches assume that $\mathbf{x}$ is k-sparse, i.e. only k of its N components are nonzero, and the sketching matrix is based on an expander construction with $m = \mathcal{O}(k \log(N/k))$ rows. In this paper, we consider structured sparsity models and show that it is possible to recover several interesting structured sparsity models using expander-based sketches with significantly fewer number of rows. We also introduce a model-based recovery framework and show that robust recovery is possible without increasing the computational cost. To obtain our results, we use a novel technique that adds a conditional probability argument to the usual probabilistic construction of expanders.

Precisely, we consider three classes $\mathcal{M}_k$ of structured signals and denote the signals belonging to these classes as *k-model sparse*, where k is a model parameter. These structures consist of a) k-rooted connected signals which have their k nonzero components lie in a rooted connected tree; b) k-block sparse signals whose support consists of k equal size non-overlapping blocks; and c) k-group sparse signals whose support is contained in the union of k overlapping groups. Note that the *sparsity* is k in model class a), but $kg_{\max}$ in model classes b) and c) where $g_{\max}$ is the maximum group size.

Our main result is to *probabilistically* design sparse binary matrices, named *model-based expanders*, that capture the structure of the signals under consideration and allow for a reduction in the storage complexity to $O(N)$ and above all, allow robust recovery with fewer measurement: $m = O(k)$ for model class a) and $m = \mathcal{O}(kg_{\max} + k \log(M/k))$ for model class b) and c), where M is the number of blocks/groups. These results hinge on a novel analysis technique based on conditional probabilities that allows to consider a wide

variety of models.

Moreover, in order to recover k-model sparse or compressible signals, we propose a modification of the popular sparse matching pursuit compressed sensing algorithm. The proposed algorithm yields an approximation $\hat{\mathbf{x}}$ with the following error guarantee (referred to as ℓ_1/ℓ_1 guarantee) in the *for all* case (when a given sketching matrix and a recovery algorithm pair achieve this error for all $\mathbf{x} \in \mathcal{M}_{\mathbf{k}}$)

$$\|\hat{\mathbf{x}} - \mathbf{x}_{\mathcal{S}}\|_1 \leq C\sigma_{\mathcal{M}_k}(\mathbf{x})_{\mathbf{1}} + \frac{\mathbf{D}}{\mathbf{d}}\|\mathbf{e}\|_{\mathbf{1}} \ ,$$

for some constants $C, D > 0$, where

$$\sigma_{\mathcal{M}_k}(\mathbf{x})_{\mathbf{1}} := \min_{\mathbf{k}-\text{model sparse } \mathbf{x}'} \|\mathbf{x} - \mathbf{x}'\|_{\mathbf{1}}.$$

The algorithm runtime complexity crucially depends on the cost of projecting onto the model $\mathcal{M}_k$. However, we show that the projections for the considered models can be computed exactly in $\mathcal{O}(Nk)$ time for model class a), at worst $\mathcal{O}\left(N\log(N)\right)$ time for model class b) and $\mathcal{O}\left(M^2k\right)$ time for a special case of the model c).

Stabilised finite element methods for a bending moment formulation of the Reissner-Mindlin plate model

Gabriel R. Barrenechea & Tomás Barrios & Andreas Wachtel *(University of Strathclyde)*

We study the stabilisation of a mixed formulation applied to Reissner-Mindlin plate model. After introducing the stress tensor as an extra unknown, a weak formulation is derived and its well-posedeness proved. Then, with the aim of using the lowest order possible finite element spaces we introduce a stabilised formulation. The advantages of this formulation are, at least, twofold. First, it allows the use of standard nodal finite element methods while keeping stability and convergence, hence avoiding the use of enriched finite element methods (like PEERS). This generates an obvious gain in terms of degrees of freedom. Also, the formulation (combined with the choice of finite element spaces) allows to impose the symmetry of the stress tensor strongly, then avoiding the introduction of a Lagrange multiplier to achieve this. Using approximation properties of the corresponding subspaces, we deduce the optimal rates of convergence. Finally, we present numerical examples confirming the theoretical properties of this approach.

A method for solution of linear inverse problem with nonlinear regularization term

Marta M. Betcke, Simon Arridge & Lauri Harhanen *(University College London)*

In this talk we present a method for solution of a large scale linear inverse problem regularized using penalty term which depends on the solution

$$\min_f \frac{1}{2}\|g - Af\|^2 + \tau f^T M_f f.$$

Such class of regularizers includes for instance the widely used total variation and Perona-Malik penalties. Important examples of linear inverse problems requiring nonlinear regularization are deblurring problems in imaging processing or fluorescense diffuse optical tomography (FDOT) in medical imaging. In particular in the latter application one seeks to reconstruct a three dimensional fluorophore distribution typically with an order of a million degrees of freedom from a comparable number of measurements. The system matrix derives from the sensitivity relation for FDOT problem, thus it is large and dense, rendering direct solution of the corresponding normal equations infeasible.

In the proposed scheme the nonlinearity is handled with the lagged diffusion iteration [1]. At each step of the nonlinear iteration we have to solve the linear problem

$$(A^TA + \tau M_{f_{k-1}})f_k = A^Tg, \tag{9}$$

which is obviously also large and dense. Hence, it has to be solved with iterative methods. Unfortunately, the convergence of Krylov methods (in particular LSQR) for such problems is rather slow. We propose to accelerate the convergence using the idea of priorconditioning of Krylov spaces. Priorconditioning is a way of incorporating the information contained in the prior M_f, which would otherwise take a long time to build up in the Krylov space, directly into the system matrix and amounts to solution of the following preconditioned system

$$(L^{-1}A^TAL^{-T} + \tau I)f_k = L^{-1}A^Tg, \quad M_{f_{k-1}} = LL^T. \tag{10}$$

In our method the preconditioning is performed implicitly, hence there is no need to factorize the preconditioner, $M_{f_{k-1}} = LL^T$. This allows for using more efficient and flexible preconditioning techniques like for instance multigrid. We demonstrate the effectiveness of the method on an example of a three dimensional FDOT problem using algebraic multigrid preconditioner.

High Order Nonlinear Diffusion: A Moving Mesh Finite Difference Method

Nicholas Bird *(University of Reading)*

We examine the fourth order nonlinear diffusion equation

$$u_t = (u^n q_x)_x, \qquad q = -u_{xx},$$

on the time dependent domain $x \in (a(t), b(t))$. We outline a velocity-based method of solution to this PDE in a moving framework. The method uses a local conservation of mass principle and maintains scale invariance.

The evolution of the time dependent domain is determined by a deformation velocity $v(x,t)$ which is determined using the local conservation of mass principle. The solution $u(x,t)$ is then recovered algebraically on the evolved domain.

We introduce a moving mesh finite difference scheme based on the method for use in obtaining numerical solutions. The scheme has the property that when $n = 1$ and initial conditions are sampled from an exact similarity solution at the nodes the approximation matches the exact solution at the nodes for all time to within rounding error. For this purpose a scale-invariant time stepping scheme is used.

The effect of choosing $n \neq 1$ on the method is highlighted and possible extensions to the method are briefly discussed.

Solving the neutron transport equation within a diffusive regime

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

We consider iterative methods for solving the neutron transport equation. This equation governs the behaviour of neutrons within a reactor and describes the behaviour of the *neutron flux* denoted $\psi(\mathbf{r}, \Omega)$, where $\mathbf{r} \in V \subset \mathbb{R}^3$ is the neutron's location in a 3D coordinate system (V is a bounded spatial domain) and $\Omega \in \mathbb{S}^2$ (the unit sphere in $\mathbb{R}^3$) is its direction of travel. The quantity $\psi(\mathbf{r}, \Omega)$ is then the number of neutrons passing through a unit space at $\mathbf{r}$ in direction Ω per unit time. The transport equation describes the behaviour of the neutron flux based upon the probabilities of various neutron interactions (or collisions) occurring, and based on the characteristics of a *neutron source*. When modelling a nuclear reactor, it is generally specified that neutrons can undergo three types of interaction: they can cause *fission*, can be *scattered* or they can be *captured*. We define the *absorption cross-section* to be the probability of either a capture or fission interaction occurring, and denote this σ_A. We will however not include fission interactions in this talk. We denote by σ_S the *scattering cross-section*, which is the probability that a neutron is scattered and ends up travelling in a new direction. We denote by σ_T the *total cross-section*, which is the probability of any collision occurring, and which satisfies $\sigma_T = \sigma_S + \sigma_A$. The *neutron source* term will be denoted by $Q(\mathbf{r})$ and is a non-fission source term, isotropic in angle, of neutrons from position $\mathbf{r}$. Under this notation, the transport equation has the following form:

$$\Omega \cdot \nabla\psi(\mathbf{r}, \Omega) + \sigma_T \psi(\mathbf{r}, \Omega) = \frac{\sigma_S}{4\pi} \int_{\mathbb{S}^2} \psi(\mathbf{r}, \Omega)\Omega + Q(\mathbf{r}), \qquad \mathbf{r} \in V, \;\; \Omega \in \mathbb{S}^2 \tag{11}$$

subject to suitable boundary conditions on the boundary of V. Alternatively it can be written abstractly in operator form:

$$\mathcal{T}\psi = \mathcal{S}\psi + Q. \tag{12}$$

Although highly non-symmetric, this equation has an equivalent symmetric integral equation formulation. Using this formulation it can be proved that if σ_S is considerably smaller than σ_T, then a simple fixed-point iteration involving repeated solves with $\mathcal{T}$ converges quickly.

In this work we focus on the case when σ_S/σ_T is close to 1. This is equivalent to the mean free path, i.e. the average distance travelled by a neutron between successive collisions, being small when compared to a characteristic length of the spatial domain. An asymptotic analysis in this case, and based on some additional assumptions, shows that the transport equation is well approximated by a certain diffusion equation. In the talk we will also investigate ways of using the diffusion approximation as a preconditioner for solving the transport equation in the diffusive regime.

Comparison of Multigrid Methods for the Solution of Nonlinear Diffusion Equations: Nonlinear vs. Newton

Keeran J Brabazon & Peter K Jimack & Matthew E Hubbard *(University of Leeds)*

Nonlinear multigrid methods have been used successfully to solve systems of nonlinear equations. There exists little convergence theory for these methods, particularly for nonlinear diffusion equations where the nonlinearity occurs in the diffusion coefficient. Previous work by one of the authors solves highly nonlinear systems of phase-field equations using implicit time stepping and nonlinear multigrid (the Full Approximation Scheme (FAS) of Brandt [1]) to solve the nonlinear equations arising at each time step [2]. This has motivated the question as to what makes multigrid methods appropriate for nonlinear diffusion problems,

and which multigrid methods will perform best for the solution of such problems.

In this presentation three different nonlinear multigrid methods are compared: (a) the Nonlinear Multilevel Method due to Hackbusch [3]; (b) a Newton-Multigrid method; and (c) a Newton-Krylov method where the Krylov subspace method is preconditioned using multigrid. To highlight the strengths and weaknesses of these methods applied to nonlinear diffusion equations the following model problems, for varying right hand side f, are investigated:

$$\begin{aligned} -\nabla \cdot \left(\left\{ 1 + \alpha (\nabla u)^2 \right\} \nabla u \right) = f, \quad x \in \Omega \equiv (0,1)^2 \\ u = 0, \quad x \in \partial\Omega \end{aligned} \tag{13}$$

and

$$\begin{aligned} -\nabla \cdot \left(\left\{ 1 + \alpha u^2 \right\} \nabla u \right) = f, \quad x \in \Omega \equiv (0,1)^2 \\ u = 0, \quad x \in \partial\Omega, \end{aligned} \tag{14}$$

with $(\alpha \geq 0) \in \mathbb{R}$. Various parameters are tuned to optimize each method, and these solution methods are compared in terms of robustness and efficiency (i.e. execution times). Issues encountered due to the properties of the underlying PDEs are considered, and recommendations on the choice of multigrid solver will be made. The presentation will end with a discussion on how these results may provide insight into how a nonlinear multigrid algorithm is likely to perform for other problems involving nonlinear diffusion.

[1]A. Brandt. *Multilevel Adaptive Solutions to Boundary Value Problems.* Mathematics of Computation, 31(138):333-390, 1977

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On the evaluation complexity of constrained smooth optimization

Coralia Cartis & Nick Gould & Philippe Toint *(University of Edinburgh)*

We propose a new termination criteria suitable for potentially singular, zero or non-zero residual, least-squares problems, with which cubic regularization variants take at most $\mathcal{O}(\epsilon^{-3/2})$ residual and Jacobian evaluations to drive either the Euclidean norm of the residual or its gradient below ϵ; this is the best-known bound for potentially rank-deficient nonlinear least-squares problems. We then apply the new optimality measure and cubic regularization steps to a family of least-squares merit functions in the context of a target-following algorithm for nonlinear equality-constrained problems; this approach yields the first evaluation complexity bound of order $\epsilon^{-3/2}$for nonconvexly constrained problems when higher accuracy is required for primal feasibility than for dual firstorder criticality. We extend our results to also include the evaluation complexity of least-squares problems with convex inequality constraints and to the general nonlinear inequality and equality constrained optimization problem.

Asymptotic analysis of interior transmission eigenvalues for a perfect conducting body coated by a thin dielectric layer

Nicolas Chaulet & Fioralba Cakoni & Houssem Haddar *(University College London)*

A new eigenvalue problem, the so-called interior transmission eigenvalue problem (ITEP), appeared in the nineteen eighties in the context of inverse scattering problems. The interior transmission eigenvalues are related to non scattering frequencies. More precisely, when such eigenvalue exists for a given dielectric object, it corresponds to a frequency for which there exists an incident wave that almost does not scatter. Recently, it has been noticed that these eigenvalues may be computed from multi static far field data and therefore they can be used for non destructive testing of materials.

We focus in this talk on the ITEP related to the scattering by an object which is a perfectly conducting body modelled by an open bounded domain Ω_δ, which is coated by a thin dielectric layer of thickness δ. We denote Ω the domain that corresponds to the union of Ω_δ and the thin layer. The corresponding ITEP writes: find $k_\delta > 0$ such that there exists a non trivial solution (w_δ, v_δ) to the following coupled problem

$$\begin{cases} \Delta w_\delta + k_\delta^2 n^2 w_\delta = 0 \quad \text{in } \Omega \setminus \overline{\Omega_\delta}, \\ \Delta v_\delta + k_\delta^2 v_\delta = 0 \quad \text{in } \Omega, \\ \dfrac{\partial v_\delta}{\partial \nu} = \dfrac{\partial w_\delta}{\partial \nu}, \quad v_\delta = w_\delta \quad \text{on } \partial\Omega, \\ w_\delta = 0 \quad \text{on } \partial\Omega_\delta \end{cases} \tag{15}$$

where n denotes the refractive index of the layer and ν denotes the outward unit normal to Ω. Existence of such eigenvalues has been proven in for small index of refraction of the coating. We go further in understanding the problem by providing a rigorous asymptotic development of the first transmission eigenvalue with respect to δ up to the second order. We finally prove that this eigenvalue problem can be approximated by an eigenvalue problem for the $-\Delta$ operator in Ω with Robin (or classical impedance) boundary condition.

The Closest Point Method and Multigrid solvers for elliptic equations on surfaces

Yujia Chen & Colin Macdonald *(University of Oxford)*

This talk concerns the numerical solution of elliptic partial differential equations posed on general smooth surfaces by the Closest Point Method. Based on the closest point representation of the surface, we formulate an embedding equation in a narrow band surrounding the surface, then discretize it using standard finite differences and interpolation schemes. In order to solve the resulting large sparse linear systems, we propose a specific geometric multigrid method which makes use of the closest point representation of the surface.

High Order Block Implicit Multistep (HOBIM) Methods for the Solution of Stiff Ordinary Differential Equations

J. P. Chollom G.M.Kumleng & S.Longwap *(University of Jos)*

The Search for higher order A-stable linear multi-step methods has been the interest of many numerical analyst and has been realised through either through higher derivatives of the solution or inserting additional off step points ,supper future points and the likes. These methods are suitable for the solution of stiff differential equations which exhibit characteristics that place severe restriction on the choice of step size. It becomes necessary that only methods with large regions of absolute stability remain suitable for these kind of equations. In this paper, high order block implicit multi-step methods of the hybrid form up to order twelve have been constructed using the multi-step collocation approach. This is achieved by inserting one or more off step points. The accuracy and stability properties of the new methods are investigated and are shown to yield A-stable methods, a property desirable of methods suitable for the solution of stiff ODEs. The new high order block implicit multi-step methods used as block integrators tested on stiff systems of ODEs reveal that they compete favorably with the state of the art Matlab ode23 code.

Multi Level Monte Carlo Methods for Atmospheric Dispersion Modelling

Sarah Cook, Rob Scheichl & Eike Mueller *(University of Bath)*

The fast and accurate prediction of the transport and spread of airborne pollutants is important both for atmospheric research and in emergency response applications, such as during the eruption of the Eyjafjallajkull volcano in 2010, which caused widespread disruption to European air travel.

The Met. Office's dispersion model (NAME) currently uses standard Monte Carlo particle methods to simulate unresolved turbulence in the atmosphere. However, the slow convergence of such methods often restricts the accuracy with which predictions can be provided on operational time scales. Multilevel Monte Carlo methods have shown great promise in other application areas, such as mathematical finance, to reduce the variance and thus allow for more complex scenarios to be modeled in a shorter time [Giles, Operations Research 56(3): 607-617, 2008]. Loosely speaking, the computational cost is reduced by computing a large number of cheap but inaccurate samples to reduce statistical noise and by then correcting these results with the refinements from more accurate (and more computationally expensive) samples to reduce the bias.

The SDEs describing the transport and dispersion of atmospheric pollutants have a very similar structure to those encountered in mathematical finance and we will present both numerical and analytical results which demonstrate the effectiveness of the multilevel approach for an Ornstein-Uhlenbeck process, which can be used as simplified model equation for homogenous atmospheric turbulence. We also investigate the performance of the multilevel method for a more realistic scenario which describes the transport and spread of pollutants in a moderate-wind neutral boundary layer.

On the volume integral equation in electromagnetic scattering

Martin Costabel & Eric Darrigrand & Hamdi Sakly *(Universit de Rennes 1)*

Formulating the scattering of electromagnetic waves by a penetrable object in the frequency domain via a volume integral equation is quite popular with physicists. There exist even widely used numerical codes based on this formulation ("discrete dipole approximation"), but the mathematical analysis is far from complete. The volume integral equation, sometimes called Lippmann-Schwinger equation, is a strongly singular integral equation, and it still poses interesting mathematical problems of a basic nature, even for the simple case of piecewise constant coefficients. In the talk, results about the essential spectrum of the volume integral operator will be presented, with emphasis on methods that work for non-smooth (Lipschitz) boundaries. It turns out that there is a way to transform the strongly singular integral equation into an equivalent coupled system of weakly singu-

lar volume integral equations and boundary integral equations such that the question of Fredholmness is reduced to that of well-known scalar boundary integral operators. A previous method of reduction to a coupled system of volume/boundary integral equations [1] led to a system of boundary integral equations that allowed a simple analysis only for smooth domains.

[1] M. Costabel, E. Darrigrand, H. Sakly: On the essential spectrum of the volume integral operator in electromagnetic scattering. *C. R. Acad. Sci. Paris*, Ser. I **350** (2012) 193–197.

Optimal Scaling Parameters for RBF-FD Aproximation of Poisson Equation

Oanh Thi Dang, Oleg Davydov & Hoang Xuan Phu *(Thai Nguyen University of Information and Communication Technology)*

We investigate the influence of the scaling parameter of the *radial basis functions (RBF)* in the meshless RBF-FD method with irregular centres for solving the Poisson equation. Numerical experiments show that the optimal scaling parameter strongly depends on the RBF and the test problem, but insignificantly on the density of the centres. Therefore, we develop an algorithm to compute effectively a near-optimal scaling parameter, which is based on comparison of RBF solutions on nested sets of centres. As result, we can obtain solutions of the PDE with accuracy comparable to those computed by linear finite elements on the same discretisation centres and with comparable density/bandwith of the system matrix.

Numerical Solution of Monge-Ampère Equation on Domains Bounded by Piecewise Conics

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

We introduce new C^1 polynomial finite element spaces for curved domains bounded by piecewise conics using Bernstein-Bézier techniques. These spaces are employed to solve fully nonlinear elliptic equations. Numerical results for several test problems for the Monge-Ampère equation on domains of various smoothness orders endorse theoretical error bounds given previously by K. Böhmer.

Remarks on two integral operators and numerical methods for Cauchy Singular Integral Equations

Maria Carmela De Bonis *(University of Basilicata)*

In [1], the mapping properties of the singular integral operator

$$(D^{\alpha,-\alpha}f)(x) = (\cos\pi\alpha)v^{\alpha,-\alpha}(x)f(x) - \frac{\sin\pi\alpha}{\pi}\int_{-1}^{1} f(y)\frac{v^{\alpha,-\alpha}(y)}{y-x}dy,$$

where $v^{\alpha,-\alpha}(x) = (1-x)^{\alpha}(1+x)^{-\alpha},\ 0<\alpha<1$, is a Jacobi weight, have been studied in Zygmund spaces equipped with uniform norm. In [2], using such properties, numerical methods for solving the following well-known Cauchy singular integral equation (CSIE) of index 0

$$(D^{\alpha,-\alpha} + K^{\alpha,-\alpha})f(x) = g(x), \tag{16}$$

where $K^{\alpha,-\alpha}$ is a compact perturbation, have been proposed when $\frac{1}{2} \le \alpha < 1$.

In this talk, the author, first will extend the above mentioned mapping properties in larger Zygmund spaces and, then will propose two quadrature methods for solving (**??**) that are stable and convergent for any choice of the parameter $0 < \alpha < 1$. Error estimates in Zygmund norm will be given and some numerical tests will be shown.

The following Cauchy equation of index 1

$$(D^{-\alpha,\alpha-1} + K^{-\alpha,\alpha-1})f(x) = g(x)$$

$$\int_{-1}^{1} f(x)v^{-\alpha,\alpha-1}(x)dx = 0,$$

will be also considered.

[1] G. Mastroianni, M. G. Russo, W. Themistoclakis: *The boundedness of a Cauchy integral operator in weighted Besov type spaces with uniform norms*, Integral Equations Operator Theory, 42 (2002), no. 1, 57–89.
[2] M. C. De Bonis, G. Mastroianni: *Direct methods for CSIE in weighted Zygmund spaces with uniform norm*, Riv. Mat. Univ. Parma., 2 (2011), 29-55.

A multilevel sparse kernel-based stochastic collocation finite element method for elliptic problems with random coefficients

Zhaonan Dong & Emmanuil H Georgoulis *(University of Leicester)*

A stochastic collocation finite element method for the numerical solution of elliptic boundary value problems (BVP) with random coefficients, based on multilevel sparse-kernel based quadrature, is proposed. Assuming that the randomness is governed by a finite number of random variables with given probability distri-

butions, the elliptic problem is transformed to its respective high-dimensional representation on the product of the BVP solution and probability spaces.

The method for solving the problem consists of a finite element approximation in the physical space, along with a collocation technique for the approximation of the integrands of the integrals in the probability space. The collocation technique is based on the *Multilevel Sparse Kernel-Based Interpolation (MLSKI)* recently presented in [E.H.Georgoulis, J.Levesley & F.Subhan, Multilevel sparse kernel-based interpolation. SIAM Journal on Scientific Computing 35(2) pp. A815A831 (2013)], which can be viewed as a sparse-grid-type algorithm based on radial-basis functions for the interpolation dimensional functions. Consequently, the method solves uncoupled deterministic problems on each collocation point.

Numerical examples show the effectiveness of this algorithm. In particular, it demonstrates at least algebraic convergence with respect to the total number of collocation points in up to 11 dimensions.

Optimisation and conditioning in variational data assimilation

Adam El-Said & N.K. Nichols, A.S. Lawless *(University of Reading)*

Data assimilation combines observations with a dynamical model of a system. The aim is to estimate the most likely state of the system given the observations. Data assimilation is an essential tool used in numerical weather prediction (NWP) to obtain accurate weather forecasts. It is cyclic in that it is applied at fixed time intervals (6 or 12 hours in the context of NWP) and the beginning of each cycle incorporates the previous forecast. This previous forecast is known as the 'background'. Statistical errors in the observations and the background are assumed to be independent and follow a Gaussian distribution. Variational data assimilation incorporates these errors into a non-linear, least-squares objective function that is constrained by the flow of the dynamical model. Four-dimensional variational data assimilation (4DVAR) seeks the optimal least-squares fit of the model trajectory to the observations over a fixed time interval, known as the 'assimilation window'. The underlying assumption in 4DVAR is that the dynamical model is perfect.

The relaxation of the 'perfect model' assumption gives rise to 'model error'. The errors in the model are also assumed to have Gaussian statistics. Therefore the objective is now to find an optimal estimate of the states across the assimilation window, given the error statistics in the background, observations and the model. This is known as *weak-constraint* 4DVAR. There are two formulations of the weak-constraint problem, which possess some interesting characteristics and properties. One formulation aims to estimate the optimal states at each time in the assimilation window. The alternative aims to estimate the optimal initial state and simultaneously the 'model error adjustments' for the assimilation window.

We are interested in using gradient-based iteration procedures to find the optimal estimate of the states. We gain insight into the accuracy and 'uniqueness' of the solution and the speed of the iterative solver by studying the condition of the Hessian of the objective function. Theoretical bounds on the L_2 condition number of the Hessian are derived here and demonstrated using a simple one-dimensional linear advection model on a periodic domain. We present numerical results to illustrate the effect of correlation length-scales, variances and observation configurations on the conditioning of the problem. We also discuss some fundamental differences between both formulations and plans for future work.

Preconditioning Technique of Darcy's Law in Porous Media

Faisal Fairag & Hattan Tawfiq & Mohammed Alshahrani *(KFUPM)*

We consider the solution of system of linear algebraic equations which is obtained from Raviart-Thomas mixed finite element formulation of Darcy's equations. In [C.E. Powell and D. Silvester, Optimal Preconditioning for Raviart-Thomas Mixed Formulation of Second-Order Elliptic problems, SIAM J. Matrix Anal. Appl., 25(2003), pp. 718-738.], Powel and Silvester developed a block-diagonal preconditioner for this system. In this research work, we extend their results by constructing a block-triangular preconditioner and establish an eigenvalue bound for the preconditioned matrix. Several numerical tests confirm the theoretical results. The preconditioned matrix is nonsymmetric but it is self-adjoint in a nonstandard inner product. A new method related to the Bramble-Pasiak Conjugate Gradient method (BPCG) is introduced. Moreover, a bound on the norm of the residual is studied. Numerical experiments illustrate good convergence properties yielding a constant number of iterations versus problem size.

Loosely Coupled Parallel Computation of Leading Part Singular Value Decomposition

Sheng Fang & Raphael Hauser *(University of Oxford)*

The development of multicore processors and graphic cards presents huge opportunities for scientific computing. As fundamental techniques and tools, new numerical linear algebra algorithms based on loosely coupled parallelism(low synchronicity, low communication overhead) are strongly desirable. In this talk, we present such an algorithm for computation of leading part singular value decomposition of very large, not necessarily sparse, matrices. Theoretical analysis and uses in several optimisation models are discussed.

RBF Multiscale Collocation for Second Order Elliptic Boundary Value Problems

Patricio Farrell & Holger Wendland *(University of Oxford)*

In this talk, we discuss multiscale radial basis function collocation methods for solving elliptic partial differential equations on bounded domains. The approximate solution is constructed in a multi-level fashion, each level using compactly supported radial basis functions of smaller scale on an increasingly fine mesh. On each level, standard symmetric collocation is employed. A convergence theory is given, which builds on recent theoretical advances for multiscale approximation using compactly supported radial basis functions.

If time permits, we also discuss the condition numbers of the arising systems as well as the effect of simple, diagonal preconditioners. In particular, we present results that prove previous numerical observations made by Fasshauer. More than a decade ago, he observed:

- There is no convergence in the stationary setting, i.e. if the support radius at a given level is chosen proportional to the mesh norm of that level.
- There is convergence, if the support radii go slower to zero than the mesh norms.
- In contrast to pure interpolation, even in the stationary setting, the condition numbers of the collocation matrices depend on the level.
- In the stationary case, a simple preconditioning $PAP = Py$ with a diagonal matrix P leads to a level-independent condition number.
- This preconditioning technique does not lead to a level-independent condition number in the non-stationary setting, where convergence occurs.

A Class of L-Stable Implicit Trapezoidal-Like Integrators for the Solution of Parabolic Partial Differential Equations on Manifolds

Johnson Oladele Fatokun & Philip Iyakino Akpan *(Federal University)*

A new Trapezoidal-type scheme is proposed for the direct numerical integration of time-dependent partial differential equations. This evolving system is usually stiff, so it is desirable for the numerical method to solve it to have good properties concerning stability. The method proposed in this article is L-stable and at least of algebraic order three. It is increasingly common to encounter partial differential equations (PDEs) posed on manifolds, and standard numerical methods are not available for such novel situations. Here an L-Stable implicit Trapezoidal-like numerical integrator was developed for solving Partial Differential Equations on manifolds. This approach allows the immediate use of familiar finite difference methods for the discretization and numerical solution. Presented here are the motivation and details of the method, illustration of its numerical convergence and stability properties for a general case. Numerical experiments illustrate the performance of the new method on different stiff systems of ODEs after discretizing in the space variable some PDE problems.

On the matrix algebra of Lorentz transformations

Roger Fletcher *(University of Dundee)*

The Lorentz transformation plays an important part in the theory of special and general relativity, and in Maxwell's equations. It has some interesting properties from a matrix algebra viewpoint which are explored in the talk. The various innovative predictions of special relativity are usually explained in terms of a simple 1+1 (one time and one space) dimensional model of spacetime. However there is an elegant general approach in 1+3D spacetime in terms of a Lorentz matrix L which satisfies the matrix equation $L^T JL = J$ where J is the so-called Minkowski metric $J = \mathrm{diag}(-1, 1, 1, 1)$. This talk shows exactly how the general case can be reduced to the simple case, which is usually only hinted at in the literature. The outcome is somewhat unexpected, and some interesting properties of the matrix L are discovered along the way. These include a generalised Cayley transformation, and simple ways of computing the Singular Value Decomposition and the Polar Decomposition. The geometrical interpretation of the reduction process is explained.

Branching and Bounding Improvements for Lipschitz Global Optimization

Jaroslav Fowkes & Coralia Cartis & Nicholas I. M. Gould *(University of Edinburgh)*

We present improved bounding procedures in the context of a recent global optimization algorithm based on cubic regularization. The bounding procedures are general and can be applied to any branch and bound algorithm that uses estimates of the spectrum of the Hessian or derivative tensor, as they are constructed using generalisations of Gershgorin's theorem and other spectral approaches.

In order to improve the branching aspects of the algorithm, and using the proposed bounding procedures, we develop parallel variants based on both data parallel and task parallel paradigms and address important performance issues that arise such as doubling of work and load balancing. Numerical testing of the bounding techniques and parallel approaches on a HPC cluster is presented with promising results.

Stabilization of convection-diffusion problems by Shishkin mesh simulation. Recent developments.

Bosco García-Archilla *(Universidad de Sevilla)*

Shishkin mesh simulation is a novel technique to stabilize numerical methods for convection-diffusion problems. It is based on simulating that the grid is the coarse part of a Shishkin grid, although it can be applied on problems where Shishkin meshes are difficult to build, including domains with nontrivial geometries. The technique, which does not require adjusting any parameter, has been shown in [1] to outperform a good deal of methods of choice today in tests that include exponential and characteristic layers, interior layers, domains with curved boundaries and convection with vortices. The tests in [1], however, concentrate on strongly convection-dominated problems. Also, in [1] the technique was developed only for linear finite-elements. In the present talk we comment on the extension to higher-order methods as well as its application to problems with moderate convection.

[1] B. García-Archilla, Shishkin mesh simulation: A new stabilization technique for convection-diffusion problems, *Comput. Methods Appl. Mech. Engrg.*, **256** (2013), 1–16.

Generalized Arnoldi-Tikhonov Methods with Applications to Sparse Reconstruction.

Silvia Gazzola *(University of Padova)*

This talk is focussed on the regularization of large-scale discrete linear ill-posed problems by means of Krylov subspace methods.

In the framework of the Arnoldi-Tikhonov methods, a new algorithm employed to solve problems of the form

$$\min_{x\in\mathbb{R}^N} \left\{\|Ax-b\|_2^2+\lambda\|L(x-x_0)\|_2^2\right\}$$

is introduced. No restrictions on the regularization matrix L are made. In order to choose the regularization parameter λ, a new efficient scheme based on the discrepancy principle is presented.

Two strategies that generalize the previous approach and that can be applied to solve problems of the form

$$\min_{x\in\mathbb{R}^N} \left\{\|Ax-b\|_2^2+\lambda\|x\|_p^p\right\}$$

and

$$\min_{x\in\mathbb{R}^N} \left\{\|Ax-b\|_2^2+\lambda \mathrm{TV}(x)\right\}$$

are addressed. The first one involves flexible preconditioning of the underlying Krylov subspaces, the second one involves suitable restarts of the Arnoldi algorithm.

Numerical examples arising from the discretization of integral equations and image restoration are given in order to show the effectiveness of these new methods; comparison with some other existing algorithms are made.

This is a joint work with Paolo Novati (Univeristy of Padova, Italy) and James Nagy (Emory University, Atlanta, USA).

An Off-step Discretization for the Solution of Two-space Dimensional Second Order Quasilinear Hyperbolic Equations

Venu Gopal & R. K. Mohanty *(University of Delhi)*

In this paper, we propose a new high accuracy numerical method of order two in time and four in space directions based on off- step discretization for the solution of two-space dimensional second order quasilinear hyperbolic partial differential equations of the form

$$u_{tt} = A(x,y,t,u)u_{xx} + B(x,y,t,u)u_{yy} + g(x,y,t,u,u_x,u_y,u_t),$$

$0 < x, y < 1$, $t > 0$ subject to appropriate initial and Dirichlet boundary conditions. We use only five evaluations of the function g and do not require any fictitious points to discretize the differential equation. The proposed method is directly applicable to wave equation in polar coordinates and when applied to a linear telegraphic hyperbolic equation is shown to be unconditionally stable. Numerical results are provided to illustrate the usefulness of the proposed method.

A practical dual gradient-projection method for large-scale, strictly-convex quadratic programming

Nick Gould, Jonathan Hogg & Jennifer Scott *(STFC-Rutherford Appleton Laboratory)*

We consider solving a given large-scale strictly convex quadratic program by applying the well-known accelerated gradient-projection method to its dual. While this might seem at first sight to be inadvisable since the dual Hessian is defined in terms of the inverse of the primal one, it turns out that all operations may be performed very efficiently so long as a sparse Cholesky factorization of the primal Hessian may be found. In particular, the gradient-projection part of each iteration requires a sequence of "Cholesky forward solves" with sparse right-hand sides, while the acceleration part may be achieved using, for example, a suitably preconditioned conjugate gradient method. Much use is made of the Fredholm alternative. We illustrate performance of this approach on standard large-scale QP examples, and highlight the method's use for warm-starting. A new fortran package DQP will shortly be available as part of GALAHAD.

Matrix-Free Physics-Based Preconditioned Krylov Subspace Methods for 2D Particle Transport Problem

Tong-Xiang Gu, Yan-Hua Cao & Xing-Ping Liu *(Institute of Applied Physics and Computational Mathematics)*

Source iteration is a iterative process usually used to solve the particle transport problem. For physical system containing subregions that are optically thick and scattering-dominated, most of the particles undergo many collisions before being captured or leaking out, source iteration is inefficient and costly. In this paper, we consider the popular preconditioned Krylov subspace method. We show how to formulate the total linear system in the discrete-ordinates and how to choose the physics-based preconditioners. To avoid too much large memory storage for coefficient matrix and preconditioners, we adopt a matrix-free technique. By this technique, the memory (excluding a few more memory for vectors's storage) needed in the preconditioned Krylov method is as much as that of the source iteration. Numerical experiments show the number of iteration and CPU time for convergence of the preconditioned BiCGSTAB methods are much less than that of source iteration for the physical system containing subregions that are optically thick and scattering-dominated. In these difficult cases, the preconditioned Krylov methods can be a quantity faster than source iteration, while for simple physical system where most of the particles undergo few collisions, source iteration is not a bad choice.

Energy Law and Its Numerical Preservation for Quasi-Incompressible Navier-Stokes Cahn-Hilliard (NSCH) System with Variable Density

Zhenlin Guo & Ping Lin & John Lowengrub *(University of Dundee)*

We will present some recent work on phase-field model for multiphase complex fluids. A Quasi-Incompressible NSCH System, which obeys the energy law for variable density, will be considered. A C^0 finite element method is designed for solving the coupled nonlinear system, in which the energy law for the system can be preserved accurately at the discrete level. Some numerical results will be presented to demonstrate the effectiveness of our numerical schemes and to validate the robustness of the quasi-incompressible NSCH.

Symmetric General Linear Methods

Adrian Hill & John Butcher *(University of Bath)*

The talk considers symmetric general linear methods, a class of numerical time integration methods which, like symmetric Runge–Kutta methods, are applicable to general time–reversible differential equations, not just those derived from separable second–order problems. A definition of time–reversal symmetry is formulated for general linear methods, and criteria are found for the methods to be free of linear parasitism. It is shown that symmetric parasitism–free methods cannot be explicit, but a method of order 4 is constructed with only one implicit stage. Several characterizations of symmetry are given, and connections are made with G–symplecticity. Symmetric methods are shown to be of even order. A suitable symmetric starting method is constructed and shown to be essentially unique. The underlying one–step method is shown to be time–symmetric. Several symmetric methods of order 4 are constructed and implemented on test problems. The methods are efficient when compared with Runge–Kutta methods of the same order, and invariants of the motion are well–approximated over long time intervals.

Tropical Eigenvalues

James Hook & Françoise Tisseur *(University of Manchester)*

Tropical eigenvalues can be used to approximate the order of magnitude of the eigenvalues of a classical matrix or matrix polynomial. This approximation is

useful when the classical eigenproblem is badly scaled. For example

$$A = \begin{bmatrix} 10^5 & -104 \\ i & 10^{-2} \end{bmatrix}, \quad Val(A) = \begin{bmatrix} 5 & 4 \\ 0 & -2 \end{bmatrix}.$$

The classical matrix A has eigenvalues $\lambda_1 = (-1 + 0.000001i) \times 10^5$ and $\lambda_2 = (-0.01 - i) \times 10^{-1}$. By taking the componentwise-log-of-absolute-value A corresponds to the max-plus matrix Val(A), which has tropical eigenvalues $t\lambda_1 = 5$ and $t\lambda_2 = -1$. In this talk I will give an overview of the theory of tropical eigenvalues for matrices and matrix polynomials emphasising the relationship between tropical and classical spectra.

Space-Time Residual Distribution Schemes on Moving Meshes

Matthew E Hubbard & Domokos Sármány & Mario Ricchiuto *(University of Leeds)*

The residual distribution framework was developed as an alternative to the finite volume approach for approximating hyperbolic systems of conservation laws which would allow a natural representation of genuinely multidimensional flow features. The resulting algorithms are closely related to conforming finite elements, but their structure makes it far simpler to construct nonlinear approximation schemes, and therefore to avoid unphysical oscillations in the numerical solution. They have been successfully applied to a wide range of nonlinear systems of equations, producing accurate simulations of both steady and, more recently, time-dependent flows.

When designed carefully, these schemes have some very useful properties. Firstly, they can be simultaneously second order accurate (in space and time) and free of unphysical oscillations, even in the presence of turning points in the solution. Secondly, the CRD (Conservative Residual Distribution) formulation [1] provides a very natural way to approximate balance terms in a manner which automatically retains equilibria inherent in the underlying system. Finally, when extended to support a discontinuous representation of the dependent variables [2], allowing discontinuities in time yields schemes which are unconditionally positive [3], *i.e.* they are free of unphysical oscillations whatever size of time-step is taken. Discontinuities in space provide a natural framework for approximating shocks and applying weak boundary conditions.

This presentation will focus on space-time residual distribution schemes and ongoing work to develop unconditionally positive schemes for approximating multidimensional, time-dependent problems. The first part of the talk will outline schemes which combine second order accuracy with unconditional positivity and numerical results will be presented for the scalar advection equation and the shallow water equations (for which the "well-balanced" property is also satisfied in the presence of source terms representing variable bed topography). This will be followed by a summary of progress in the application of these schemes on adaptive, moving, meshes.

[1] Á. Csík, M. Ricchiuto, H. Deconinck, *A conservative formulation of the multidimensional upwind residual distribution schemes for general nonlinear conservation laws*, J Comput Phys, 179(2):286–312, 2002.
[2] M.E. Hubbard, *Discontinuous fluctuation distribution*, J Comput Phys, 227(24):10125–10147, 2008.
[3] D. Sármány, M.E. Hubbard, M. Ricchiuto, *Unconditionally stable space-time discontinuous residual distribution for shallow-water flows*, submitted to J Comput Phys (INRIA Report RR-7958).

Least Squares $h-p$ Spectral Element Methods for Boundary Layer Problems on Nonsmooth Domains

Akhlaq Husain *(LNM Institute of Information Technology)*

Boundary layers arise as solution components in singularly perturbed elliptic boundary value prob- lems in the study of plates and shells in structural mechanics and in heat transfer problems with small thermal coefficients. Serious efforts have been made in the literature for resolution of bound- ary layers and the approximation theory and convergence results for singularly perturbed problems on smooth domains have been well established in late 90'ties within the framework of finite dif- ference methods and finite element methods. In case of non-smooth domains such as domains with corners, in addition to the corner singularities, the boundary layers arise which are solution components in a narrow neighborhood of the boundary of the domain. Due to the presence of singularities, the approximation becomes difficult and the conventional numerical methods fail to provide accurate solutions to the boundary layer problems on non-smooth domains. It is known that the solution to a singularly perturbed boundary value problem on non-smooth domains can be decomposed into a smooth part, a corner layer part and a boundary layer part. In this presentation we propose a least-squares $h-p$ spectral element method which will approximate the solution to boundary layer problems on non-smooth domains with exponential accuracy using parallel computers. To resolve the boundary layers and corner singularities we use local systems of coordinates. These local coordinates (auxiliary mappings) are modified version of polar coordinates. Away from the corners standard Cartesian

coordinates are used. In the neighbourhoods of corners we use a geometrical mesh which becomes finer towards the corners. The geometrical mesh becomes a quasi-uniform mesh in the new system of coordinates. We then derive differentiability estimates in these new set of variables and a stability estimate on which our method is based for a non- conforming $h-p$ spectral element method. A parallel preconditioner to solve the normal equations is defined, using the stability estimates.

Fourth Order Variational Formulation for Image Registration

Mazlinda Ibrahim & Ke Chen *(University of Liverpool)*

Registration is a crucial task in image processing particulary in medical imaging, target tracking, motion estimation and satellite imagery. It seeks to find the optimal transformation, so that the template image becomes similar to the so-called given reference image. In order to compute a transformation which matches given images, two main components are combined. Firstly, there must be a similarity measure to quantify the extent to which a transformation has achieved the matching goal. A common similarity measure in mono-modal image registration is the sum of the squared difference (SSD). Secondly, to overcome the ill posed nature of registration problem, a measure of transformation regularity is required. Typically, the desired transformation is determined by minimising an energy functional consisting of a weighted sum of these two measures. Several first order regularisation terms have been proposed to seek for a smooth transformation but the models require an affine linear pre-registration. In order to remove the dependency to the pre-registration step, second order term is used in the regularisation part which do not penalize rigid transformation. In this talk, I shall introduce to the two second order regularisation terms in image registration model which are Fischer and Modersitzki (2003)'s curvature term that is linear and mean curvature by Chumchob, Chen and Brito (2011) that is highly nonlinear. In the variational formulations setting, the minimiser is characterised by fourth order Euler Lagrange equations. Numerical scheme will employ to the discrete Euler Lagrange equations that require a fast algorithm to solve the problem. Some results for both models will be presented using multigrid method and brief discussion for multi-modal image registration.

A Parallel Solver for the Forward Problem in Electrical Impedance Tomography using DUNE FEM

Markus Jehl, Timo Betcke, Andreas Dedner & David Holder *(University College London)*

Electrical Impedance Tomography is an established method to image changes of conductivity in geometrically simple objects. The structure of the head complicates the measurement of impedance changes within the brain, as most of the applied current does not pass the brain, but is diverted through the scalp and cerebrospinal fluid (CSF) layers. Because only a small portion of the injected current will actually flow through the brain, we have a small signal-to-noise ratio. This imposes strong precision requirements on both, the instrumentation and the modeling.

To our knowledge it has not yet been analysed scientifically, how precise the forward model (i.e. the finite element mesh (FEM) of the head) needs to be, in order to detect changes in conductivity within the brain. To study these precision requirements we need to have a numerical solver which can quickly solve the simplified (static) Maxwell's equations on the FEM of the head. By parallelisation we can segment the FEM into several parts which will then be computed on a group of processors. For our solver we used the C++ library DUNE FEM, which provides a good framework of classes and functions that facilitate the creation of a FEM solver supporting MPI, adaptive mesh refinement and more.

Using the broadly accepted complete electrode model for the modeling of the electrodes, our Poisson problem takes the following shape in the weak formulation

$$\int_\Omega \sigma \nabla v \nabla u + \sum_{l=1}^{L} \frac{1}{z_l} \int_{\Gamma_l} vu - \sum_{l=1}^{L} \frac{1}{z_l |\Gamma_l|} \int_{\Gamma_l} v \int_{\Gamma_l} u = \sum_{l=1}^{L} \frac{1}{|\Gamma_l|} \int_{\Gamma_l} v I_l,$$

where L is the number of electrodes, Γ_l is the surface of electrode l, z_l is the contact impedance, I is the input current and σ the conductivity.

Having the simulated voltage distributions, we are looking at optimal current patterns for different meshes using the distinguishability measure

$$\|v_e(\sigma_1, j) - v_e(\sigma_2, j)\| / \|j\| > \epsilon, \tag{17}$$

which can also give us an idea of the measurement precision that is required to distinguish two different conductivity distributions. Here, $v_e(\sigma_1, j)$ denotes the resulting electrode voltages for a conductivity distribution σ_1 when a current j is applied. By finding the Neumann-to-Dirichlet map this leads to a generalised eigenvalue problem on the surface mesh, which needs to be solved efficiently.

A posteriori error analysis for fully discrete Crank – Nicolson schemes

Fotini Karakatsani, Eberhard Bänsch & Charalambos Makridakis *(University of Strathclyde)*

We derive residual-based a posteriori error estimates of optimal order for fully discrete approximations for linear parabolic problem. The time discretization uses the Crank–Nicolson method and the space discretization uses finite element spaces that are allowed to change in time. The main tool in our analysis is the comparison with an appropriate reconstruction of the discrete solution.

Application of Preconditioned Conjugate Gradient Method to Some Challenging Large Scale Problems in Computational Geomechanics

Omid Kardani, Andrei V. Lyamin & Kristian Krabbenhoft *(University of Newcastle, Australia)*

The application of convex programming in solving optimization problems arising in Geomechanics has recently been of growing interest and significant advances have been made in this field. Some of the most important applications in Geomechanics include traditionally difficult problems in plasticity, limit and elastoplastic analysis and most recently granular contact dynamics, which we focus on in this paper. This problem can be formulated as convex programming, particularly second order conic programming (SOCP). Upon formulating the original problem as SOCP, it can be efficiently solved by primal-dual interior point method (IPM).

In each step of this method, in order to update the current optimum point, a Newton search direction vector needs to be calculated by solving a symmetric positive definite (SPD) linear system of equation which is usually highly ill-conditioned. Due to their robustness and accuracy, the direct solvers have been traditionally used for this task. However, for large three dimensional problems direct solvers require prohibitively high storage and computational efforts. Therefore, the use of iterative solvers becomes imperative. But iterative schemes are often far from being accurate for highly ill-conditioned systems. This motivates using appropriate preconditioners to enhance the efficiency of the iterative solution schemes.

In our study, we use preconditioned Conjugate Gradient method (PCG) with the most popular incomplete factorization preconditioning techniques in the framework of IPM method and address the implementation challenges, such as efficient choice of stopping criteria for both outer and inner iterations, the preconditioner based on the current solution approximate and other parameters related to the PCG method.

Furthermore, some large scale sample geotechnical problems are solved by our proposed algorithm and the results are discussed. Finally, some comments on the methods which can improve the efficiency of the iterative solution schemes are provided and some suggestion for future research in the field is presented, particularly in terms of parallel computation.

LU factorization with panel rank revealing pivoting

Amal Khabou, James W. Demmel, Laura Grigori & Ming Gu *(University of Manchester)*

We present a block LU factorization with panel rank revealing pivoting (block LU_PRRP), an algorithm based on strong rank revealing QR for the panel factorization. Block LU_PRRP is more stable than Gaussian elimination with partial pivoting (GEPP), with a theoretical upper bound of the growth factor of $(1 + \tau b)^{(n/b)-1}$, where b is the size of the panel used during the block factorization, τ is a parameter of the strong rank revealing QR factorization, and n is the number of columns of the matrix. For example, if the size of the panel is $b = 64$, and $\tau = 2$, then $(1 + 2b)^{(n/b)-1} = (1.079)^{n-64} \ll 2^{n-1}$, where 2^{n-1} is the upper bound of the growth factor of GEPP. Our extensive numerical experiments show that the new factorization scheme is as numerically stable as GEPP in practice, but it is more resistant to some pathological cases where GEPP fails. We note that the block LU_PRRP factorization does only $O(n^2 b)$ additional floating point operations compared to GEPP.

Numerical solution of fourth order parabolic partial differential equation using exponential sextic splines

Arshad Khan and Pooja Khandelwal *(Jamia Millia Islamia)*

In this paper, we report three level implicit method of high accuracy schemes of $O(k^4+h^6)$ and $O(k^4+h^8)$ for the numerical solution of fourth order variable coefficient non-homogeneous parabolic partial differential equation, that governs the behaviour of a vibrating beam. Exponential sextic spline is used in space and finite difference discretization in time. The linear stability of the presented method is investigated. It has been shown that by suitably choosing the parameters most of the previous known methods for homogeneous and non-homogeneous cases can be derived from our method. The presented methods are tested on two

examples. The computed results are compared wherever possible with those already available in literature. This shows the superiority of the presented method.

Local Estimates of the Time-Stepping Error for High-Order Splitting Methods

Othmar Koch & W. Auzinger, H. Hofstätter, and M. Thalhammer *(Vienna University of Technology)*

We discuss the structure of the local error of high-order split-step time integrators for nonlinear evolution equations of Schrödinger type in both a semi-discrete and fully discretized setting,

$$\dot{u} = F(u), \quad F(u) = Au + B(u),$$

where $A = \mathrm{i}\Delta$ and B is a generally unbounded, nonlinear operator. Based on a rigorous analysis of the error structure which is detailed for a Laguerre–Fourier–Hermite spatial discretization for a rotating Bose–Einstein condensate, we introduce estimators for the local error and prove their asymptotical correctness. The estimators are based on embedded formulae for the method coefficients or alternatively on the defect correction principle. The resulting time-stepping strategies are demonstrated to reflect the solution behavior well. Finally we assess the strategies' efficiency by numerical comparisons.

A New Splitting Method and its Analysis for Non-autonomous Systems

Sıla Övgü Korkut & Gamze TanoĞLU *(Izmir Katip Çelebi University)*

Operator splitting methods have been extensively applied to solve complicated systems of differential equations. In this process we split the complex problem into several sub-problems, each of which can be solved sequentially. In this study, we develop a new operator splitting method combining the iterative idea which involves Magnus expansion. We also investigate its convergence properties by using the concepts of stability, consistency, and order for both linear and nonlinear non-autonomous systems. Several numerical examples are illustrated to confirm the theoretical results by comparing frequently used methods.

A New Fifth-Order Derivative Free Newton-type Method for Solving Nonlinear Equations

Manoj Kumar & Akhilesh Kumar Singh & Akanksha Srivastava *(Motilal Nehru National Institute of Technology)*

In the present paper, we are concerned with a new fifth order convergent Newton-type iterative method with and without derivative for estimating a simple root of the nonlinear equations. The error equations are used to establish the fifth order of convergence of the proposed iterative methods. Finally, various numerical comparisons are made using MATLAB to demonstrate the performance of the developed methods.

How to compute the reflection and transmission coefficients of a plane acoustic wave by a low-porosity perforated plate ?

S Laurens, E. Piot, A Bendali, M Fares, & S Tordeux *(CERFACS)*

Perforated plates and screens are widely used in engineering systems due to their ability to absorb sound or to reduce sound transmission, in a variety of applications including room acoustics and aeroacoustics. They can be used as protective layers of porous materials, to form sandwich structures in aircraft fuselages or as facing layers of liners. In this case, the perforated plates are either backed by honeycomb cells which are mounted on a rigid backplate or by a plenum acting as a resonant cavity in gas turbine combustion chambers.
In this work, we investigate the acoustic properties of a low-porosity perforated plate in a compressible ideal inviscid fluid in the absence of mean flow. Because the acoustic wavelength is large as compared with the aperture size, each aperture can be considered as acoustically compact. This means that the local motion through an aperture is assumed to be incompressible. At a large enough distance from the perforated plate, the scattered pressure field can be decomposed into a reflected and a transmitted wave where the reflection and transmission coefficients are complex constants, depending on the acoustic properties of the plate. In particular, we show that they can be expressed in terms of the Rayleigh conductivity of an isolated perforation by extending the approach introduced for the case of thick plates by [1]. The Rayleigh conductivity depends on the ratio of the volume flux through the aperture by the difference in unsteady pressure between each sides of the plate. Using the linearized momentum equation, it can be expressed as a function of pressure only, but it still require the computation of the solution to obtain its value. For thin plates with a circular aperture, [2] gives an analytical expression of this quantity. For untilted cylindrical or conical apertures, one only have the Howe'estimates [3], established empirically by assuming that the flow is potential and governed by the linearized Helmholtz equation in the aperture if the characteristic size of the hole is small in comparison with the acoustic wavelength.

Lower and upper bounds for the Rayleigh conductivity of a perforation in a thick plate are usually derived from intuitive approximations and by reasoning based on physical observation like Howe's. This work addresses a mathematical justification of these approaches, yielding accurate bounds for various geometries, untilted or tilted, with a conical shape or an elliptical section. Accurate estimates of the Rayleigh conductivity for a single perforation have a direct impact on the precision of models used for predicting the acoustic behavior of a perforated plate mainly on the basis of its reflection and transmission coefficients. It'll be shown in this work how asymptotic expansions can be used to derive first and second-order accurate, albeit approximate expressions of these coefficients, as well as of the effective compliance of the perforated plate.

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On the evaluation of some integral operators with Mellin type kernel

Concetta Laurita *(University of Basilicata)*

We consider the numerical evaluation of integral transform of the form

$$(\mathcal{K}f)(y) = \int_0^1 \frac{1}{x} k\left(\frac{y}{x}\right) f(x)dx, \quad y \in (0,1], \qquad (18)$$

for some given function $k : [0,\infty) \to [0,\infty)$ satisfying suitable assumptions. These operators of Mellin convolution type are not compact and their kernels are not smooth but contain a fixed strong singularity at $x = y = 0$.

The mathematical formulation of many problems in physics and engineering gives rise to the solution of second kind integral equations involving operators of the form (**??**). When we are interested in the numerical solution of such equations by means of Nyström or discrete collocation methods, efficient quadrature formulas are necessary, in order to approximate the integrals $(\mathcal{K}f)(y)$, $y \in (0,1]$.

The aim of this talk is to propose an algorithm for the evaluation of these integrals, since the fixed singularity of the Mellin kernel at the origin makes inefficient the use of the classical Gaussian rules when y is very close to the endpoint 0.

Covariance Structure Regularization via Entropy Loss Function

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

The need to estimate structured covariance matrices arises in a variety of applications and the problem is widely studied in statistics. We propose a new method for regularizing the covariance structure of a given covariance matrix, in which the underlying structure is usually blurred due to random noises particularly when the dimension of the covariance matrix is high. The regularization is made by choosing an optimal structure from an available class of covariance structures in terms of minimizing the discrepancy, defined via the entropy loss function, between the given matrix and the class. A range of potential candidate structures such as tridiagonal, compound symmetry, AR(1), and Toeplitz are considered. Simulation studies are conducted, showing that the proposed new approach is reliable in regularization of covariance structures. The approach is also applied to real data analysis, demonstrating the usefulness of the proposed approach in practice.

On the computational modelling of cell migration and chemotaxis

John Mackenzie & Michael Nolan & Matt Neilson & Steve Webb & Robert Insall *(University of Strathclyde)*

A computational framework is presented for the simulation of eukaryotic cell migration and chemotaxis. An empirical pattern formation model, based on a system of non-linear reaction-diffusion equations, is approximated on an evolving cell boundary using an Arbitrary Lagrangian Eulerian surface finite element method (ALE-SFEM). The solution state is used to drive a mechanical model of the protrusive an retractive forces on the cell boundary. Movement of the cell is achieved using a parameterised finite element method. Results are presented for cell migration with and without chemotaxis. The simulated behaviour is compared with experimental results of real cells.

Adaptive discontinuous Galerkin methods for non-stationary convection-diffusion problems

Stephen Metcalfe *(University of Leicester)*

This talk is concerned with the derivation of a robust a posteriori error estimator for a discontinuous Galerkin method discretisation of a linear non-stationary convection diffusion initial/boundary value problem and with the implementation of a corresponding adaptive algorithm. More specifically, we derive a posteriori bounds for the error in the $L^2(H^1) + L^\infty(L^2)$-type norm for an interior penalty discontinuous Galerkin (dG) discretisation in space and a backward Euler discretisation in time. An important feature of the estimator is robustness with respect to the Péclet number of the problem which is verified in practice by a series of numerical experiments. Finally, an adaptive algorithm is proposed utilising the error estimator. Optimal rate of convergence of the adaptive algorithm is observed in a number of test problems.

Algorithmic and Parallel Scalability of Elliptic Solvers in Atmospheric Modelling

Eike Hermann Mueller & Robert Scheichl *(University of Bath)*

Semi-implicit time stepping is very popular and widely used in numerical weather- and climate prediction models for various reasons, particularly since it allows for larger time steps and thus for better efficiency. However, the bottleneck in semi-implicit schemes is the need for a three dimensional elliptic solve for the pressure correction in each time step. With increasing model resolution this elliptic PDE can only be solved on operational timescales if highly efficient algorithms are used and their performance and scalability to large problem sizes can be guaranteed on massively parallel computers.

We have studied both the elliptic PDE in the ENDGame dynamical core of the Unified Model and a typical model equation arising from semi-implicit semi-Lagrangian time stepping; problems with a similar structure are encountered in other areas of geophysical modelling, such as ocean circulation models and subsurface flow simulations. In particular, the vertical extent of the domain is significantly smaller than the horizontal size and one of the defininining characteristics of elliptic PDEs encountered in geophysical applications is a strong anisotropy in the vertical direction. To take this into account, these equations are usually discretised on grids with a tensor-product structure with a unstructured (or semi-structured) horizontal mesh and a regular grid for each vertical column. We implemented a bespoke, geometric multigrid solver based on [Börm S., Hiptmair R., Numer. Algorithms 26: 2001. (1999)] which exploits the grid structure and strong vertical anisotropy.

We demonstrated the algorithmic scalability of a tensor-product multigrid solver based on the latitude dependent semi-coarsening approach in [Buckeridge S, Scheichl R., Numerical Linear Algebra with Applications 17(2-3): 325-342 (2010)] for the pressure correction equation in the ENDGame dynamical core and compared it to the current one-level method (BiCGStab preconditioned with vertical line relaxation). For the model equation on grids with a tensor product structure we showed the superior performance of our matrix-free geometric multigrid algorithm which avoids precomputation of the matrix and coarse grid setup costs. We compared our method to existing AMG solvers from the DUNE and Hypre libraries and demonstrated its performance both in terms of absolute solution time and parallel scalability as well as its robustness for systems with more than 10^{10} degrees of freedom on up to 65536 CPU cores of the HECToR supercomputer.

Computing the common zeros of two bivariate functions via Bézoutians

Vanni Noferini & Yuji Nakatsukasa, Alex Townsend *(University of Manchester)*

The real common zeros of two bivariate functions can be computed by finding the common zeros of their polynomial interpolants expressed in a tensor Chebyshev basis. From here we develop a bivariate rootfinder based on the hidden variable resultant method and Bézout matrices. Using techniques such as domain subdivision, regularization of the Bézout matrix polynomial, spurious roots analysis, and a local Bézout rootfinding routine, we are able to accurately compute the simple common zeros of two smooth functions to essentially machine precision. As a result, we can efficiently deal with high-degree (100 or more), dense bivariate polynomials. Our robust algorithm is designed to be compatible with Chebfun2, a software package written in object-oriented MATLAB for computing with bivariate functions. More details on Chebfun2 will be given in Alex Townsend's talk.

This is joint work with Yuji Nakatsukasa (Manchester/Tokyo) and Alex Townsend (Oxford).

A Fresh Start For Leapfrog

Terence Norton *(University of Bath)*

The Leapfrog method has the structure-preserving properties of time-symmetry & G-symplecticity, which are desirable for the long–time numerical integration of Hamiltonian systems. However, in common with other explicit linear multistep methods, it is prone to parasitism. In this talk, we investigate the role that start-

ing methods can play in triggering or suppressing parasitism. We study the effects of using

- A conventional Euler starter;
- A starter which respects time–symmetry;
- An iterative starter which eliminates parasitic components at $t = 0$.

A Dicontinuous Galerkin Approach for Flows in Porous Media

F.Z. Nouri & A. Assala *(Adji Mokhtar University)*

This paper is devoted to the numerical analysis study of the coupled system of Navier-Stokes and Darcy equations by means of the Beavers-Joseph-Saffman's condition on the interface. This model is discretized using the discontinuous Galerkin finite element method in the whole domain. We prove a *priori* and a *posteriori* error estimates for the resulting discrete problem. Some numerical experiments confirm the interest of the discretization.

Approximation of Hadamard finite-part integrals on the semiaxis

Donatella Occorsio & Maria Carmela De Bonis *(University of Basilicata)*

Hadamard finite-part integrals of type

$$=\int_0^\infty \frac{f(x)}{(x-t)^2}\, w_\alpha(x)dx,$$

where $w_\alpha(x) = e^{-x}x^\alpha,\ \alpha > 0$, is a Laguerre weight, are of interest in the numerical approximation of hypersingular integral equations on the half-plane by using a BEM approach as discretization technique (see [1]).

To our knowledge, most of the papers available in the literature deal with the approximation of Hadamard integrals on bounded intervals (see for instance [3] and the references therein). On the other hand, in the case of semifinite integrals, the existing procedures make use of suitable transformation to bounded intervals (see [1], [2]).

In this talk we propose two numerical methods for approximating Hadamard integrals (**??**). The proposed procedures use the global approximation based on the zeros of Laguerre orthogonal polynomials. We prove that they are stable and convergent in suitable weighted uniform spaces and give some error estimates. Finally, we show the performance of the procedures by some numerical tests.

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Regularity of the solution to a class of nonlinear weakly singular integral equations

Arvet Pedas & Gennadi Vainikko *(University of Tartu)*

The differential properties of a solution to a nonlinear weakly singular Uryson type integral equation are examined. Showing that the solution belongs to a special weighted space of functions, the growth of its derivatives near the boundary of the interval of integration is described. We extend the corresponding results of [1],[3] to a wider class of nonlinear weakly singular integral equations having point singularities. In the linear case similar results are obtained in [2].

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IIPBF - a Matlab toolbox for computing infinite integrals of products of Bessel functions of the 1st and 2nd kind

Tilak Ratnanather *(Johns Hopkins University)*

A MATLAB toolbox, IIPBF, for calculating infinite integrals involving a product of two Bessel functions ($J_a(\rho x)J_b(\tau x)$, $J_a(\rho x)Y_b(\tau x)$ or $Y_a(\rho x)Y_b(\tau x)$) for non-negative a, b and a kernel $f(x)$, has been developed and applied to several test cases. Based on a Fortran algorithm previously developed for $J_a(\rho x)J_b(\tau x)$ only, the toolbox first expresses the product as a sum of fast and slow oscillating components and implements a three step procedure of adaptive integration, summation and extrapolation. IIPBF utilizes customized functions from SLATEC library conversion together with quadgk, an adaptive Gauss-Kronrod quadrature. The applicability of IIPBF to problems in fluid mechanics and imaging science suggest its functionality

can be expanded to consider spherical Bessel functions, real valued a, b and complex valued kernel. Attention will be paid to the problem of dealing with the first two zeros of one component which can affect the performance of quadgk.

A meshfree method for elasticity problems with interfaces

Magda Rebelo & Nuno Martins *(Universidade Nova de Lisboa and CEMAT-Instituto Superior Técnico)*

In this talk, we propose a meshfree method based on fundamental solutions basis functions for a transmission problem in linear elasticity. The addressed problem consists in, given the displacement field on the boundary, compute the corresponding displacement field of an elastic object (which has piecewise constant Lamé coefficients) . The Lamé coefficients are assumed to be constant in non overlaping subdomains and, on the corresponding interface (interior boundaries), non homogeneous jump conditions on the displacement and on the traction vectors are considered. The main properties of the method are analyzed and illustrated with several numerical simulations in 2D and 3D domains.

Higher Fréchet derivatives of Matrix Functions and Applications

Samuel D. Relton & Nicholas J. Higham *(University of Manchester)*

For a matrix function $f\colon \mathbb{C}^{n\times n} \mapsto \mathbb{C}^{n\times n}$ we can define its Fréchet derivative $L_f(A,E) \in \mathbb{C}^{n\times n}$ to be the unique linear function that satisfies $f(A+E) = f(A) + L_f(A,E) + o(\|E\|)$ for any E. The Fréchet derivative has been applied in matrix optimization, model reduction, image registration and cancer analysis. Another use for the Fréchet derivative is to define the condition number of a matrix function (how sensitive $f(A)$ is to perturbations in A), which is a measure of how accurately we can compute $f(A)$ in floating point arithmetic.

This talk describes some potential applications for higher order Fréchet derivatives: in particular we use the second Fréchet derivative to investigate the condition number of computing a Fréchet derivative and the level-2 condition number of a matrix function(sensitivity of the condition number to perturbations in A). The latter in particular seems an interesting area for future research and shows complicated interaction

Construction of robust and efficient Implicit-Explicit Runge-Kutta methods

T. Roldán & I. Higueras *(Universidad Pública de Navarra)*

Space discretization of some time-dependent PDEs gives rise to systems of ordinary differential equations in additive form

$$y' = f(y) + g(y)\,, \qquad y(t_0) = y_0\,, \tag{19}$$

where $f, g : \mathbb{R}^k \to \mathbb{R}^k$ are sufficiently smooth functions with different stiffness properties. In these cases, implicit methods should be used to treat the stiff terms while efficient explicit methods can still be used for the nonstiff part of the equation.

In this work we study different implicit-explicit Runge-Kutta methods for additive differential equations of the form (**??**). In the construction of Runge-Kutta methods, properties like stability and accuracy should be taken into account. However, in some contexts, storage requirements of the schemes play an important role. Low storage explicit Runge Kutta methods have been studied by some authors [1],[2],[4],[5] in different contexts. Some analysis for IMEX methods can be seen in [3].

In this study we construct different implicit-explicit Runge-Kutta methods with good stability properties and low storage requirements.

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Numerical methods for Fredholm integral equations defined on the square

Maria Grazia Russo & Donatella Occorsio *(University of Basilicata)*

We deal with the numerical approximation of the solution of Fredholm integral equations of the second

kind, defined on the square $S = [-1, 1]^2$,

$$f(x, y) - \mu \int_S k(x, y, s, t) f(s, t) w(s, t)\, ds\, dt = g(x, y), \tag{20}$$

where $w(x, y) := v^{\alpha_1,\beta_1}(x) v^{\alpha_2,\beta_2}(y) = (1 - x)^{\alpha_1}(1 + x)^{\beta_1}(1 - y)^{\alpha_2}(1 + y)^{\beta_2}$, $\alpha_1, \beta_1, \alpha_2, \beta_2 > -1$, $\mu \in \mathbf{R}$. k and g are given functions defined on $[-1, 1]^4$ and $[-1, 1]^2$ respectively, which are sufficiently smooth on the open sets but can have (algebraic) singularities on the boundaries. f is the unknown function.

Some of the existing numerical procedures for solving (**??**) make use of collocation or Nyström methods based on piecewise approximating polynomials or Montecarlo methods, or discrete Galerkin methods.

In our talk, following a well known approach in the one dimensional case, we propose a global approximation of the solution by means of a Nyström method based on a cubature rule obtained as the tensor product of two univariate Gaussian rules and a polynomial collocation method, both based on Jacobi zeros. The reasons why this approach is not trivial is that there are very few results in the literature about the polynomial approximation in two variables.

Moreover the additional difficulty of considering functions which can have singularities on the boundaries can be treated only by introducing weighted approximation schemes and weighted spaces of functions.

We show that, under suitable assumptions on the weights, the linear systems equivalent to the proposed methods are uniquely solvable and well-conditioned. Moreover we prove that both methods are stable and convergent, giving error estimates in suitable two-dimensional Sobolev spaces, equipped with the weighted uniform norm.

A priori convergence bounds for Hermitian inexact Krylov methods for eigenspaces

Christian Schröder & Ute Kandler *(TU Berlin)*

The methods of choice for computing an invariant subspace $\mathcal{X}$ of a large sparse Matrix A are Krylov methods that search a sequence of Krylov subspaces $\mathcal{K}_k(A, v_0)$ of increasing dimension k for approximations of $\mathcal{X}$. When the matrix gets really large or rounding is involved one has to deal with *inexact* Krylov subspaces. The question arises whether Krylov methods still converge and what convergence behavior can be expected. We present a priori bounds on the angle between the invariant subspace $\mathcal{X}$ of the Hermitian matrix A and the k-th inexact Krylov subspace $\tilde{\mathcal{K}}_k$. The bound is in terms of eigenvalues of A, their gaps and uses Chebychev polynomials.

The bound constitutes a generalization of Saad's theorem [Thm 6.3 in Saad, *Numerical methods for large eigenvalue problems*, SIAM, 2011] in several respects: i) it considers invariant subspaces instead of eigenvectors; ii) it allows for inexactness in the formation of the Krylov subspaces; iii) the eigenvalues corresponding to $\mathcal{X}$ need not be well separated from the remaining spectrum of A for the bound to be useful.

The presentation is supported by numerical experiments.

On the Jacobi-collocation method for some nonlinear singular Volterra integral equations

S. Seyedallaei & T. Diogo & M. Rebelo *(Instituto Superior Técnico-Centro de Matemática e Aplicações)*

We consider a nonlinear Volterra integral equation whose solution is not differentiable at the origin. Due to this behaviour the orders of convergence of collocation and product integration methods are not optimal. After an adequate change of variables the equation can be transformed into one whose solution has better regularity properties. We show that the Jacobi-collocation method can then be applied to yield higher accurate approximate solutions. Some examples are presented which illustrate the performance of the proposed method.

Locating the Eigenvalues of Matrix Polynomials

Meisam Sharify & Dario A. Bini & Vanni Noferini *(University of Manchester)*

Some known results for locating the roots of polynomials are extended to the case of matrix polynomials. These results include a theorem by A.E. Pellet and some results based on the Newton polygon. The Newton polygon is also used in "tropical algebra" (or max-plus algebra) to compute the so-called "tropical roots" which coincide with the opposites of the slopes of the Newton polygon. It has been proved by Hadamard, Ostrowski and Pólya that the moduli of the roots of a scalar polynomial can be bounded by the "tropical roots". We extend these bounds to the case of matrix polynomials and we show that the tropical roots, which can be computed in linear time and depend only on the norms of the matrix coefficients, can provide an a priori estimation of the moduli of the eigenvalues. These extensions are applied to determine effective initial approximations for the numerical computation of the eigenvalues of matrix polynomials by means of simultaneous iterations, like the Ehrlich-Aberth method. Numerical experiments

that show the computational advantage of these results are presented.

Determinants, inverses and matrix functions: Modern iterative methods in computational statistics

Daniel Simpson *(NTNU)*

Statistical problems are getting bigger. Statistical computing, however, has some catching up to do. In the particular case of classical Bayesian modelling of spatial and spatio-temporal processes, numerical methods are almost always based around direct factorisations of covariance (and precision) matrices. When replacing these direct methods with iterative methods, the challenge comes from the types of operations that statisticians need to perform: log-determinants, traces of products of inverses, and inverse square roots of very large, ill-conditioned matrices all arise naturally. In this talk I will outline several strategies for solving these problems using a novel combination of "preconditioning" and variance reduction techniques. The trick is to remember that when "preconditioning" we do not need to compute the same number, but rather we must make sure we solve the same problem!

Krylov Subspace Recycling for Families of Shifted Linear Systems

Kirk M. Soodhalter, Daniel B. Szyld & Fei Xue *(Johannes Kepler University)*

We address the solution of a sequence of families of linear systems. For the ith family, there is a base coefficient matrix A_i, and the coefficient matrices for all systems in the ith family differ from A_i by a multiple of the identity, i.e.,

$$A_i x_i = b_i \quad \text{and} \quad (A_i + \sigma_i^{(\ell)} I) x_i^{(\ell)} = b_i \quad \text{for} \quad \ell = 1 \ldots L_i,$$

where L_i is the number of shifted systems in family i. This is an important problem arising in various applications. We extend the method of subspace recycling to solve this problem by introducing a GMRES with subspace recycling scheme for families of shifted systems. This new method solves the base system using GMRES with subspace recycling while constructing approximate corrections to the solutions of the shifted systems at each cycle. These corrections improve the solutions of the shifted system at little additional cost. At convergence of the base system solution, GMRES with subspace recycling is applied to further improve the solutions of the shifted systems to tolerance. We present analysis of this method and numerical results involving systems arising in lattice quantum chromodynamics.

Implicit methods for fractional diffusion problems

Ercília Sousa & Can Li *(University of Coimbra)*

A one dimensional diffusion problem is considered, where a fractional derivative replaces the usual second order derivative, leading to enhanced diffusion. Fractional derivatives are non-local operators opposed to the local behaviour of integer derivatives and they can be defined through the Riemann-Liouville operator. We derive a second order discretization for the Riemann-Liouville fractional derivative and then an unconditionally stable weighted average finite difference method is obtained for the diffusion equation. The stability of this scheme is established by von Neumann analysis. Some numerical results are shown, which demonstrate the efficiency and convergence of the method.

Positive solutions of semi-linear elliptic equation using finite element approximation

Akanksha Srivastava & Manoj Kumar *(Motilal Nehru National Institute of Technology)*

Numerical techniques for solving partial differential equations have been developed very fast in recent years to obtain approximate solutions for an initial or boundary value problems involving nonlinear terms in different dimensions. Present article describes the mathematical modeling and finite element approximation to study the existence and multiplicity of numerical positive solutions of logistic equation with sign-changing weight function. We investigate the range of the real parameter involve in the problem considered to achieve the numerical solutions and discuss the behavior of the branch of the solutions using MATLAB 7.0.

Evaluation and Design of Quadrature for Contour Integral Based Eigenvalue Algorithms

Allan Struthers & Stephanie Kajpust & Mark Carlson *(Michigan Technological University)*

Recent algorithms for various eigenvalue problems approximate invariant subspaces using resolvents. As an example, for the generalized eigenvalue problem $Av = \lambda Bv$,

$$P_\gamma S = -\frac{1}{2\pi i} \oint_\gamma (A - zB)^{-1} BS \, dz$$

gives the projection of a sample $S \in R^{n \times p}$ of p n-vectors onto the eigenspace associated with the generalized eigenvalues within the simple, positively-oriented contour γ. Choosing a parametrization $z(t) : 0 \leq t \leq$

1 for γ and a q point quadrature scheme (with weights $\omega_1, \omega_2, \cdots, \omega_q$ and evaluation points $0 \leq t_1 < t_2 < \cdots < t_q \leq 1$) gives the computation underlying the FEAST algorithm [1],[4]

$$P_\gamma S \approx T = -\frac{1}{2\pi i} \sum_{j=1}^{q} [\omega_j \, \text{linsol}\,(A - z(t_j)B, BS)\; z'(t_j) dt]$$

which is implemented in the recent MKL library release [5]. These algorithms adapt naturally to hierarchical parallel computer architectures. The number of independent linear solves q and the number of vectors in the sample p can be tailored to the available hardware. The preprocessing (e.g computation of a sparse LU decomposition) for each linear solve is shared by the p right handsides with the final computation being naturally embarassingly parallel.

Effective quadrature schemes are fundamental to such algorithms. If p exceeds the eigen-dimension the columns of $P_\gamma S$ span the eigenspace. An effective quadrature scheme produces columns of T which identify the eigen-dimension and produce reliable basis for the eigenspace. Current algorithms use general purpose quadrature schemes: FEAST [1],[4],[5] uses Gauss points on the upper half of real-axis-centered circular contours for real-symmetric generalized eigenproblems; Trapezoid rules on circular contours are used in [2], [3] for nonlinear eigenproblems.

This presentation introduces tools to evaluate general quadrature schemes for the specific integrations that are involved in these resolvent-based algorithms. These tools can guide the design of quadrature schemes tailored for specific algorithms. The efficacy of these schemes will be illustrated on the generalized eigenvalue problem.

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An abstract multigrid framework applied to a Stokes control problem

Stefan Takacs *(University of Oxford)*

In this talk we consider a Stokes control model problem (velocity tracking problem). The discretization of the optimality system (KKT system) characterizing the solution of such a PDE-constrained optimization problem leads to a large-scale sparse linear system. This system is symmetric but not positive definite. Therefore, standard iterative solvers are typically not the best choice. The KKT system is a linear system for two blocks of variables: the primal variables (velocity field, pressure distribution and control) and the Lagrange multipliers introduced to incorporate the partial differential equation. Based on this natural block-structure, we can verify that this system has a saddle point structure where the $(1,1)$-block and the $(2,2)$-block are positive semidefinite. Contrary to the case of elliptic optimal control problems, the $(1,2)$-block is not positive definite but a saddle point problem itself.

We are interested in fast iteration schemes with convergence rates bounded away from 1 by a constant which is independent of the discretization parameter (the grid size) and of problem parameters, like in the regularization parameter in the model problem. To achieve this goal, we propose an all-at-once multigrid approach. In the talk we will introduced an abstract framework which facilitates the construction and the analysis of all-at-once multigrid methods for block-structured problems. Based on this framework, we will discuss the choice of an appropriate smoother and sketch a convergence proof.

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Exploiting low rank of damping matrices using the Ehrlich-Aberth method

Leo Taslaman *(The University of Manchester)*

We consider quadratic matrix polynomials $Q(\lambda) = M\lambda^2 + D\lambda + K$ corresponding to vibrating systems with low rank damping matrix D. Our goal is to exploit the low rank property of D to compute all eigenvalues of $Q(\lambda)$ more efficiently than conventional methods. To this end, we use the Ehrlich-Aberth method recently investigated by Bini and Noferini for computing the eigenvalues of matrix polynomials. For general matrix polynomials, the Ehrlich-Aberth method computes eigenvalues with good accuracy but is unfortunately relatively slow when the size of the matrix polynomial is large and the degree is low. We revise the algorithm and exploit the special structure of our systems to push down the bulk sub-computation from cubic to linear time (in matrix size) and obtain an

algorithm that is both fast and accurate.

A tree projection algorithm for wavelet-based sparse approximation

Andrew Thompson & Coralia Cartis *(University of Edinburgh)*

The discrete wavelet transform is a much-used tool in digital signal processing, since it provides sparse representations for piecewise-smooth signals. Its coefficients can be naturally organized into a multi-scale tree structure, with sparse approximations typically forming rooted subtrees. We propose a dynamic programming algorithm for projection onto a sparse wavelet subtree. We prove that our algorithm has O(Nk) complexity, where N is the dimension of the signal and k is the sparsity of the tree approximation. While other recently proposed algorithms solve relaxations of the original integer program, and only give approximate tree projections for a given sparsity, our algorithm is guaranteed to compute the projection exactly. We also present the results of numerical experiments which illustrate the algorithm's efficiency.

Adaptive Discontinuous Galerkin Methods for Nonlinear Diffusion-Convection-Reaction Models

Murat Uzunca & Bülent Karasözen *(Middle East Technical University)*

Many engineering problems such as chemical reaction processes, combustion problems, transport in porous media problems arising in petroleum and ground water application are governed by coupled diffusion-convection-reaction partial differential equations (PDEs) with nonlinear source or sink terms. In the linear case, when the system is convection dominated, stabilized finite elements and discontinuous Galerkin methods are capable of handling the nonphysical oscillations. Nonlinear reaction terms pose additional challenges. Nonlinear transport systems are typically convection and/or reaction dominated with characteristic solutions possessing sharp layers. In order to eliminate spurious localized oscillations in the numerical solutions discontinuity or shock-capturing techniques are applied in combination with the streamline upwind Petrov-Galerkin(SUPG) method.

In contrast to standard Galerkin finite element methods, the discontinuous Galerkin methods produce stable solutions without need of extra stabilization techniques to overcome the spurious oscillations for convection dominated problems. In this talk we present the application of adaptive discontinuous Galerkin methods to time dependent convection dominated coupled PDEs with Monod and Arhenius type reaction rates, which occur in biodegradiation and combustion. A posteriori error estimates for linear problems in space discretization are extended to PDEs with nonlinear reaction terms. Numerical results demonstrate the accuracy and efficiency of the adaptive DGFEM compared over the SUPG and shock capturing techniques.

Product quasi-interpolation method for weakly singular integral equations

Gennadi Vainikko & Eero Vainikko *(University of Tartu)*

As a rule, the behaviour of a solution to a weakly singular integral equation with diagonal and boundary singularities is singular at the end poins of the interval. We use the well known change of variables to regularize the solution, and for the transformed equation we construct a discretization based on the collocation and a product quasi-interpolation by **smooth** splines. The method is fully discrete and of an optimal accuracy.

We pay much attention to the computation of the matrix elements in the matrix form of the method. Simple exact formulae are available, they are quite suitable for the matrix elements near the diagonal; in traditional methods difficulties appear namely here. Unfortunately, far from the diagonal, exact formulae become unstable in standard arithmetics, but there exist effective stable approximate formulae which, conversely, become inaccurate near the diagonal; approximate formulae are more labour consuming. We pay much theoretical and numerical attention to the question how far from the diagonal it is appropriate to change the exact formulae against an approximate one. In engineer computations where, say, an accuracy O(E-5) of the numerical solution is sufficient, usually all matrix elements can be computed via the exact formula using double precision arithmetics.

Numerical Integration on the Sphere using an Equal Area Mapping from the Regular Octahedron

Jan Van lent *(University of the West of England)*

A typical way of constructing numerical integration rules is to look for a set of points and corresponding weights so that a weighted average of function values at these points gives the exact result for all polynomials up to a certain degree. To avoid possible sensitivity to errors in the function values, it is important that all the weights are positive. For numerical integration on the sphere, it has been shown that it is actually possible to find spherical t-designs. These are rules

of polynomial accuracy up to degree t, where all the weights are equal. However, finding sets of points that achieve positive or equal weights using as few points as possible, requires the solution of difficult nonlinear optimisation problems. It is known that if, for a required degree of polynomial accuracy, we allow more than the minimal number of points, finding integration rules with good properties can become easier.

We introduce a method for constructing numerical integration rules based on equal area mappings from a polyhedron to the sphere. Specifically, based on an equal area mapping from the regular octahedron to the sphere, we propose a family of point sets that is very easy to generate. For these given points, we show that we can obtain weights that are positive and actually very close to being all equal. Furthermore, the weights can be computed efficiently using standard numerical linear algebra techniques, i.e., without having to resort to nonlinear optimisation. The proposed rules require more points than the standard tensor product rules for numerical integration on the sphere, but they are almost as easy to generate, the points are more evenly distributed and the weights are much closer to being all equal.

A $\mathcal{C}^0$ interior penalty method for a singularly-perturbed fourth-order elliptic problem on layer adapted meshes

Andreas Wachtel, H.-G. Roos & S. Franz *(University of Strathclyde)*

Trying to approach a fourth-order problem with a conforming method is computationally expen- sive, as finite elements need to be continuously differentiable across inter-element boundaries. The continuous interior penalty method uses standard $\mathcal{C}^0$ finite elements of degree $k \geq 2$. In order to en- sure that the finite element method has a unique solution, jumps of derivatives across inter-element boundaries are penalised. Choosing these penalties appropriately also ensures convergence.

In 2002, the method was first constructed on domains with smooth boundaries. Later, in 2005, an analysis on polygonal domains was performed. In both cases on shape-regular meshes of meshsize h and for not perturbed problems.

There are robust a-priori convergence results on shape-regular meshes of meshsize h. In the presence of layers, however, the quantities of interest $|u|_1$ and $|u|_2$, namely derivatives of first and second order, are approximated only poorly near the boundary.

As a first step to tackle this behaviour, we proved an a-priori convergence result of the CIP method on a layer-adapted mesh. Under reasonable assumptions the method convergences uniformly and of almost order $k-1$ on layer-adapted meshes. The result is of better order than the known robust result on standard meshes. A by-product of the analysis is an explicit lower bound for the penalty parameters whose choice in literature usually is a weakness of penalty methods. In this talk, we present our a-priori convergence result, a lower bound for the penalty parameter and some numerical evidence.

Preconditioning for PDE-constrained optimization

Andy Wathen *(Oxford University, UK)*

Many control problems for PDEs can be expressed as Optimization problems with the relevant PDEs acting as constraints. As is being discovered in other areas such as multi-physics, there seem to be distinct advantages to tackling such constrained Optimization problems 'all-at-once' or with a 'one-shot' method. That is, decoupling of the overall problem in some loosely coupled iterative fashion appears to be a rather poorer approach than to compute on the fully coupled problem.

The use of iterative methods for the relavant linear algebra is crucial here since the overall dimensions (including the Optimization and PDE) are usually very large, but matrix vector products as required in Krylov subspace methods such as MINRES are still readily computed. The work to ensure rapid convergence is in preconditioning and it is this topic that we will mostly focus on in this lecture.

Mathematical Deblurring of Images for Non-Blind and Blind Restoration

Bryan Williams & Ke Chen *(University of Liverpool)*

Blurring of images occurs in many fields and causes significant problems in retinal imaging. Despite significant developments in photographic techniques and technology, blur is still a major cause for image quality degradation in clinical settings. This is due to many factors such as the motion of the camera or more commonly in the case of retinal images the target scene, defocusing of the lens system, imperfections in the electronic, photographic, transmission medium, or obstructions. The age of the patient is also a relevent factor as well as pre-existing conditions.

In any diabetic retinopathy screening programme, up to 10% of the images received are ungradable due to inadequate clarity or poor field definition. It is im-

portant to obtain as much information as possible of retinal vessels and other structures in order to facilitate treatment planning or to allow further processing. Deblurring is a major technique that may be developed to restore the lost true image. This work also has applications in segmentation which aims to distinguish objects in the foreground of an image from objects in the background. There exist segmentation models which can cope well with noise but struggle with blurred images because the boundary of the object of interest is not clear.

We can place most deblurring problems into two categories. Firstly, the non-blind case [Rudin, Osher & Fatemi (1992)], where the kernel (blur function) is known and we wish to restore the image. Secondly, we have the blind case (Chan & Wong [1998]), where neither the kernel nor the image is known and we wish to recover both simultaneously. Since we usually do not know the blurring function, a significant number of problems fall into this category. Along with semi-blind restoration, these techniques are important for applications such as medical imaging, astronomical imaging and remote sensing.

In this talk, we follow the variational approach to deblurring, which leads to solving large systems of non-linear partial differential equations. Since such problems are ill-posed, the objective function must be regularized. While faster solvers are required to give efficient yet accurate results using high-order models, one particular remaining challenge is to improve the results of non-negatively constrained optimisation, which can help to improve the quality of the restored image or kernel. This is also useful for astronomical imaging and in particular for blind deblurring where the absence of positivity constraints can cause the model to fail.

For the non-blind case, we use transformations to impose positivity and hence convert the constrained problem of non-negative optimisation to a new unconstrained problem where positivity is satisfied. Such transformations are necessarily non-linear and so we employ lagging techniques and delay the linearisation until the last moment in order to keep the linear approximation of the current estimate close to the non-linear estimate. The results are competitive with Vogel and Bardsley [2002]. We aim to generalise these results to blind deconvolution where strict positivity can enhance the robustness of the results and improve on the Chan-Wong formulation.

We present some recent examples of CMIT work in this area using medical, non-medical and artificial images which have been corrupted by known blur in some cases and by unknown blur in others. In the case of known blur, we present the reconstructed images as well as some examples of reconstructed blur functions, where we assume that the true image is known, but we want to know the cause of the degredation. In the case of unknown blur, we present the reconstructed images and blur functions.

Convergence of Gravitational Search Algorithm

Anupam Yadav & Kusum Deep
(Indian Institute of Technology Roorkee)

Gravitational Search Algorithm (GSA) is a recent heuristic optimization algorithm. It is inspired by Newton's basic physical theory that a force of attraction works between every particle in the universe and this force is directly proportional to the product of their masses and inversely proportional to the square of distance between their positions. Gravitational search algorithm is successfully employed for constrained as well as unconstrained optimization problems. In the present article a proof of convergence of GSA is employed. The convergence of GSA is analytically proved with the help of recurrence relation approach.

$$vel = rand() \times vel + acceleration$$

$$pos = pos + vel$$

The velocity update equation and position update equations are considered as recurrence relation and the converging point is evaluated by solving Eq. Where acceleration is taken from the Newton's law of motion i.e. $acceleration = Force/mass$. A statistical method is employed for parameter choice involved in the GSA.

Artificial Neural Network Technique for solving Troesch's problem

Neha Yadav & Manoj Kumar *(Motilal Nehru National Institute of Technology)*

An artificial neural network approach, based on the back propagation algorithm, is presented for the numerical solution of Troesch's problem which occurs in the investigation of the confinement of a plasma column by radiation pressure. In this article, a mathematical model of the Troesch's problem arising in confinement of plasma column is presented and solved for two special cases of Eigen values using artificial neural network technique. The results of the proposed method have been compared with the analytical solutions as well as with some other existing numerical methods in the literature. It is observed that the results obtained by this method are not only more precise but also the solution is provided on continuous

finite time interval unlike the other numerical techniques. The main advantage of the proposed approach is that once the network is trained, it allows instantaneous evaluation of solution at any desired number of points spending negligible computing time and memory.

Optimal active-set prediction for interior point methods

Yiming Yan & Coralia Cartis *(University of Edinburgh)*

When applied to an inequality constrained optimization problem, interior point methods generate iterates that belong to the interior of the set determined by the constraints, thus avoiding/ignoring the combinatorial aspect of the solution. This comes at the cost of difficulty in predicting the optimal active constraints that would enable termination. We propose the use of controlled perturbations to address this challenge. Namely, in the context of linear programming with only nonnegativity constraints as the inequality constraints, we consider perturbing the nonnegativity constraints so as to enlarge the feasible set. Theoretically, we show that if the perturbations are chosen appropriately, the solution of the original problem lies on or close to the central path of the perturbed problem and that a primal-dual path-following algorithm applied to the perturbed problem is able to predict the optimal active-set of the original problem when the duality gap (for the perturbed problem) is not too small. Encouraging preliminary numerical experience is obtained when comparing the perturbed and unperturbed interior point algorithms' active-set predictions for the purpose of cross-over to simplex.

Towards the development and application of optimal solvers for continuum models of tumour growth

Fengwei Yang, Matthew E Hubbard and Peter K Jimack *(University of Leeds)*

In this talk we will present details of our development of nonlinear multigrid solvers for a variety of time-dependant systems of PDEs. Example problems will include models of thin film flows [1] and a Cahn-Hilliard-Hele-Shaw system [2]. Our goal is to develop efficient solution software that has stable second order temporal discretization based upon implicit schemes. We will demonstrate that through the use of FAS multigrid we are able to achieve second order accuracy in time and space at an optimal (O(N)) computational cost.

The second half of the talk will show ongoing work to extend these results to a phase field system for tumour growth [3], and to discuss further extensions to:

- parallel implementation,
- adaptive meshing,
- 3-D.

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Refinable C^2 Piecewise Quintic Polynomials on Powell-Sabin-12 Triangulations

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

We present a construction of nested spaces of C^2 macro-elements of degree 5 on triangulations of a polygonal domain obtained by uniform refinements of an initial triangulation and a Powell-Sabin-12 split [3]. The new refinable C^2 macro-elements have degree 5 which is substantially lower than degree 8 of the splines of [2] and degree 9 of the refinable C^2 spline spaces with stable dimension suggested in [1]. The nestedness of the spaces is achieved as in [1] by relaxing the C^3 smoothness conditions at the vertices of macro-triangles, which allows to break the 'super-smoothness disks' at the vertices into half-disks. The new macro-elements have stable local minimal determining sets (MDS) and therefore they can be used to construct nested spline spaces with stable local bases and optimal approximation power.

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On Dynamically Orthogonal Fields Approach for Time Dependent Stochastic PDEs

Tao Zhou *(Chinese Academy of Sciences, Beijing, China)*

Joint work with Prof. Fabio Nobile & Prof.Tao Tang

In this work, we first review some popular approaches for stochastic PDEs. Then, we concerned with the convergence analysis for the Dynamically orthogonal (DO) filed approach for time dependent stochastic PDEs. First, we show that the DO approach is coincide with a dynamically double orthogonal (DDO) approach, which admit a strong relationship with the dynamically SVD decomposition in the matrix context. By adopting the analysis idea of dynamically SVD decomposition by Lubich ,we show that the approximation error of DO approach can be bounded by the best low rank approximation (e.g., the truncated Karhunen-Lòeve expansion), under some reasonable assumptions. Then, by considering a simple example (the linear parabolic problem with random initial data), we show how the DO field approach works and its convergence rate. We also discuss the implementation of the numerical approaches for the resulting DO field system, on the emphasize of the case when the initial covariance matrix has singular eigenvalues. Numerical examples are provided to certify the theoretical findings.

Convexity and solvability of radial basis functions with different shapes

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

It is known that interpolation by radial basis functions with the same shape parameter can guarantee a non-singular interpolation matrix, so that solvability is ensured. Whereas little was previously known when using differing shape parameters. In this talk, we prove that a class of compactly supported radial basis functions(due to Wendland) are convex on a certain part of their support. Based on this (local) convexity and a simple local geometrical property of the interpolation points, we construct sufficient conditions which guarantee diagonal dominance interpolation matrices that arise from these radial basis functions with variate shape parameters. This proves the solvability of the radial basis function interpolation problem for these compactly supported radial basis functions with differing shape parameters and differing support. Real-word applications will be supplied to verify our results.