

22nd Biennial Conference on Numerical Analysis

26–29 June, 2007

Contents

Introduction	1
List of participants	2
Abstracts of Invited Talks	8
Abstracts of Contributed Talks	12
Timetable	40

INTRODUCTION

Welcome to the 22nd Biennial Dundee Conference.

- **General**

There will be an information/registration desk in the Foyer of the Tower Building.

- **Accommodation**

This is mainly in Belmont Hall and in Seabraes. A map of the campus is included here.

- **Meals**

All meals are in the Duncan of Jordanstone Cantina (see the map). Breakfast is available from 07.45 till 08.45, lunch from 12.50 till 13.45 and dinner from 18.30 till 19.30 (except Thursday). You should enter and leave the building by the door at the east end of the building.

- **Lecture Rooms**

These are all in the Tower Building. In addition to the main auditorium DT on the ground floor (D'Arcy Thompson Lecture Theatre), Rooms T4 and B1.36 on the first floor, and T9 on the second floor are being used. These will be signposted.

- **Chairing sessions**

Please scrutinise the timetable to see if you are down to chair a session. It is hoped that you are willing to act in this way, and this will be assumed unless we hear from you. A break of 5 minutes has been allowed for moving between rooms. Please keep speakers to the timetable so that movement to other rooms is possible for the given start times, although it may be appropriate to allow questions to continue into this period.

- **Coffee and Tea Breaks**

Coffee and tea will be provided at the advertised times in the Tower Foyer.

- **Reception**

A reception for all participants will be held in the Dundee University Students Association (DUSA) Building from 20.00 to 22.00 on Tuesday 26 June.

- **Party**

All participants are invited to a party in the DUSA Building on Wednesday 27 June from 20.00 to 22.00. Music will be provided by Ceilidh Minogue (mainly traditional Scottish music).

- **Conference Dinner**

The conference dinner will be held in the DUSA Building on Thursday 28 June, 19.30 for 20.00. The guest speaker will be Professor Nick Trefethen, University of Oxford.

- **Book displays**

Cambridge University Press and Oxford University Press will have books on display in Rooms G3 and G4 for the duration of the Conference.

Invited Speakers

Douglas Arnold	University of Minnesota arnold@ima.umn.edu	USA
Dugald Duncan	Heriot-Watt University D.B.Duncan@ma.hw.ac.uk	UK
Roger Fletcher	University of Dundee fletcher@maths.dundee.ac.uk	UK
Bengt Fornberg	University of Colorado fornberg@colorado.edu	USA
Gene Golub	Stanford University golub@stanford.edu	USA
Paul Houston	University of Nottingham Paul.Houston@nottingham.ac.uk	UK
Angela Kunoth	Universität Bonn kunoth@iam.uni-bonn.de	Germany
Jeremy Levesley	University of Leicester jl1@mcs.le.ac.uk	UK
Sven Leyffer	Argonne National Laboratory leyffer@mcs.anl.gov	USA
Volker Mehrmann	Technische Universität Berlin mehrmann@math.tu-berlin.de	Germany
David Silvester	University of Manchester d.silvester@manchester.ac.uk	UK
Zdenek Strakos	Academy of Sciences of the Czech Republic strakos@cs.cas.cz	Czech Republic
Denis Talay	INRIA denis.talay@sophia.inria.fr	France
Nick Trefethen	Oxford University LNT@comlab.ox.ac.uk	UK

Participants

Mark Ainsworth	Strathclyde University m.ainsworth@strath.ac.uk	UK
Mehiddin Al-Baali	Sultan Qaboos University albaali@squ.edu.om	Oman
Nasser Al-Salti	University of St Andrews na76@st-andrews.ac.uk	UK
Bahman Arabzadeh	Amir Kabir University arabzadeh@aut.ac.ir	Iran
Mario Arioli	Rutherford Appleton Laboratory m.arioli@rl.ac.uk	UK
Dhavid Aruliah	University of Ontario Institute of Technology Dhavid.Aruliah@uoit.ca	Canada
Noor Badshah	University of Liverpool noor.badshah@liv.ac.uk	UK
Mike Baines	University of Reading m.j.baines@rdg.ac.uk	UK
Seyed E Banifatemi	Amir Kabir University banifatemi@aut.ac.ir	Iran

Silvia Barbeiro	University of Coimbra silvia@mat.uc.pt	Portugal
Rick Beatson	University of Canterbury rick.beatson@canterbury.ac.nz	New Zealand
Jean-Paul Berrut	University of Fribourg, Switzerland jean-paul.berrut@unifr.ch	Switzerland
Timo Betcke	The University of Manchester timo.betcke@maths.man.ac.uk	UK
Marta Betcke	University of Manchester m.betcke@maths.man.ac.uk	UK
Abdellatif Bettayeb	University of Dundee latif@maths.dundee.ac.uk	UK
Bonhi Bhattacharya	University of Reading afr06bsb@reading.ac.uk	UK
Nuray Bozkaya	Middle East Technical University bnuray@metu.edu.tr	Turkey
Canan Bozkaya	Middle East Technical University bcanan@metu.edu.tr	Turkey
Hermann Brunner	Memorial University of Newfoundland hermann@math.mun.ca	Canada
Sean Buckeridge	University of Bath sdb22@bath.ac.uk	UK
Mikhail Bulatov	Siberian Branch, Russian Academy of Science mvbul@icc.ru	Russia
Corinna Burkard	University of Reading c.b.burkard@reading.ac.uk	UK
Siobhan Burke	Oxford University siobhan.burke@comlab.ox.ac.uk	UK
Coralia Cartis	Rutherford Appleton Laboratory C.Cartis@rl.ac.uk	UK
Naresh Chadha	University of Limerick naresh.chadha@ul.ie	Ireland
Graeme Chalmers	University of Strathclyde ta.gcha@maths.strath.ac.uk	UK
Mark Chaplain	University of Dundee chaplain@maths.dundee.ac.uk	UK
Bobby Cheng	The MathWorks, Inc bcheng@mathworks.com	USA
Rob Corless	University of Western Ontario rcorless@uwo.ca	Canada
Eduardo Cuesta	University of Valladolid eduardo@mat.uva.es	Spain
Penny Davies	University of Strathclyde penny@maths.strath.ac.uk	UK
Oleg Davydov	University of Strathclyde oleg.davydov@strath.ac.uk	UK
Achiya Dax	Hydrological Service dax20@water.gov.il	Israel
Sue Dollar	Rutherford Appleton Laboratory s.dollar@rl.ac.uk	UK
Iain Duff	STFC Rutherford Appleton Laboratory i.s.duff@rl.ac.uk	UK
Alan Elcrat	Wichita State University elcrat@math.wichita.edu	USA
Charlie Elliott	University of Sussex c.m.elliott@sussex.ac.uk	UK

Hind Fadel	Univeristy of Leeds indd@comp.leeds.ac.uk	UK
Faisal Fairag	KFUPM ffairag@kfupm.edu.sa	Saudi Arabia
Giovanna Fiandaca	UCL, University College London g.fiandaca@ucl.ac.uk	UK
Natasha Flyer	National Center for Atmospheric Research flyer@ucar.edu	USA
Eric Fraga	University College London e.fraga@ucl.ac.uk	UK
Sebastian Franz	TU Dresden sebastian.franz@tu-dresden.de	Germany
Melina Freitag	University of Bath m.freitag@maths.bath.ac.uk	UK
Emanuele Galligani	University of Modena and Reggio Emilia galligani@unimo.it	Italy
Mahadevan Ganesh	Colorado School of Mines mganesh@mines.edu	USA
Bosco García-Archilla	Universidad de Sevilla bosco@esi.us.es	Spain
Emmanuil Georgoulis	University of Leicester Emmanuil.Georgoulis@mcs.le.ac.uk	UK
Alf Gerisch	University of Halle alf.gerisch@mathematik.uni-halle.de	Germany
Stefano Giani	University of Bath sg240@maths.bath.ac.uk	UK
Janice Giudice	The Univeristy of Oxford Janice.Giudice@comlab.ox.ac.uk	UK
Nick Gould	Oxford University/RAL nick.gould@comlab.ox.ac.uk	UK
David Griffiths	Dundee University dfg@maths.dundee.ac.uk	UK
Sevin Gümğüm	Izmir University of Economics sevin.gumgum@ieu.edu.tr	Turkey
Nachi Gupta	University of Oxford nachi@comlab.ox.ac.uk	UK
Nick Hale	University of Oxford nicholas.hale@comlab.ox.ac.uk	UK
Julian Hall	University of Edinburgh J.A.J.Hall@ed.ac.uk	UK
Edward Hall	University of Nottingham edward.hall@nottingham.ac.uk	UK
Vjeran Hari	University of Zagreb hari@math.hr	Croatia
Alan Hegarty	University of Limerick alan.hegarty@ul.ie	Ireland
Nicholas Higham	University of Manchester higham@ma.man.ac.uk	UK
Des Higham	University of Strathclyde djh@maths.strath.ac.uk	UK
Iveta Hnetynkova	Academy of Sciences of the Czech Republic hnetynkova@cs.cas.cz	Czech Republic
Jonathan Hogg	University of Edinburgh J.Hogg@ed.ac.uk	UK
Matthew Hubbard	Univeristy of Leeds meh@comp.leeds.ac.uk	UK

Frank Hulsemann	EDF R&D frank.hulsemann@edf.fr	France
Willem Hundsdorfer	CWI willem.hundsdorfer@cw.nl	The Netherlands
Karel in 't Hout	University of Antwerp karel.inthout@ua.ac.be	Belgium
Somkid Intep	University of Strathclyde rs.sint@maths.strath.ac.uk	UK
Siraj Islam	University of Engng. and Tech., Peshawar sirajuet@yahoo.com	Pakistan
Nicolas Jeannequin	Computing Laboratory, Oxford University nicolas.jeannequin@new.ox.ac.uk	UK
Max Jensen	Durham University m.p.j.jensen@durham.ac.uk	UK
Peter Jimack	University of Leeds pkj@comp.leeds.ac.uk	UK
Phil Knight	Strathclyde University p.a.knight@strath.ac.uk	UK
Pantelis Kotzonis	Oxford University pkotzonis@hotmail.com	UK
Prashant Kumar	MNNIT, Allahabad kam3545@gmail.com	India
Jack Lambert		UK
Marko Lindner	jack.lambert@tiscali.co.uk University of Reading m.lindner@reading.ac.uk	UK
Torsten Linss	TU Dresden torsten.linss@tu-dresden.de	Germany
John Mackenzie	Strathclyde University jam@maths.strath.ac.uk	UK
Niall Madden	National University of Ireland, Galway Niall.Madden@NUIGalway.ie	Ireland
Thushka Maharaj	University of Oxford thushka.maharaj@some.ox.ac.uk	UK
Bob Marlow	University of Leeds rmarlow@comp.leeds.ac.uk	UK
William McLean	University of New South Wales w.mclean@unsw.edu.au	Australia
Angela Mihai	University of Cambridge lam40@cam.ac.uk	UK
Moss Mokgolele	University of Reading m.mokgolele@reading.ac.uk	UK
Bill Morton	Oxford morton@comlab.ox.ac.uk	UK
Nabil Nassif	American University of Beirut nn12@aub.edu.lb	Lebanon
Nancy Nichols	University of Reading n.k.nichols@rdg.ac.uk	UK
Richard Norton	University of Bath ran20@maths.bath.ac.uk	UK
Fatma Zohra Nouri	Laboratoire de Mathématiques Appliquées fz_nouri@yahoo.fr	Algeria
Dirk Nuyens	K.U. Leuven dirk.nuyens@cs.kuleuven.be	Belgium
Dion O'Neale	Massey University d.r.oneale@massey.ac.nz	New Zealand

Thomas O'Neill	Edith Cowan University t.o_neill@ecu.edu.au	Australia
Nneoma Ogbonna	Heriot Watt University N.Ogbonna@ma.hw.ac.uk	UK
George Emese Okecha	University of Fort Hare gokecha@ufh.ac.za	South Africa
Gerhard Opfer	University of Hamburg opfer@math.uni-hamburg.de	Germany
Yadollah Ordokhani	Alzahra University ordokhani@alzahra.ac.ir	Iran
Christoph Ortner	University of Oxford christoph.ortner@comlab.ox.ac.uk	UK
Ricardo Pachon	Oxford University ricardo.pachon@comlab.ox.ac.uk	UK
Manouchehr Parsaei	University of Tehran Parsaei@khayam.ut.ac.ir	Iran
Blair Perot	University of Massachusetts perot@ecs.umass.edu	USA
Maria Pickett	University of Limerick maria.pickett@ul.ie	Ireland
Cecile Piret	University of Colorado Piret@colorado.edu	USA
Martin Plesinger	Institute of Computer Science martin.plesinger@gmail.com	Czech Republic
Ana María Portillo	University of Valladolid ana@mat.uva.es	Spain
Michael Powell	University of Cambridge mjdp@cam.ac.uk	UK
Oyesetan Prince Waheed	Bright College brightcollege@alumnidirector.com	Burkina Faso
Gaurav Prinja	University of Manchester gaurav.prinja@postgrad.manchester.ac.uk	UK
Hou-Duo Qi	University of Southampton hdqi@soton.ac.uk	UK
Alison Ramage	University of Strathclyde A.Ramage@strath.ac.uk	UK
Richard Rankin	University of Strathclyde rs.ran@maths.strath.ac.uk	UK
Mohammad Rastegari	University of Shomal rastegari.mohammad@yahoo.com	Iran
Nicolette Rattenbury	Manchester Metropolitan University n.rattenbury@mmu.ac.uk	UK
Tyrone Rees	University of Oxford tyrone.rees@comlab.ox.ac.uk	UK
John Reid	Rutherford Appleton Laboratory j.k.reid@rl.ac.uk	UK
Miro Rozloznik	Czech Academy of Sciences miro@cs.cas.cz	Czech Republic
Nico Schlömer	TU Dresden nico.schloemer@gmx.net	Germany
Rene Schneider	TU-Chemnitz rene.schneider@mathematik.tu-chemnitz.de	Germany
Jennifer Scott	Rutherford Appleton Laboratory j.a.scott@rl.ac.uk	UK
Sanja Singer	University of Zagreb ssinger@fsb.hr	Croatia

Sasa Singer	University of Zagreb <code>singer@math.hr</code>	Croatia
Meghan Stephens	National University of Ireland, Galway <code>meghan.stephens@nuigalway.ie</code>	Ireland
Laura Stewart	University of Reading <code>l.m.stewart@reading.ac.uk</code>	UK
Martin Stoll	Oxford University <code>martin.stoll@comlab.ox.ac.uk</code>	UK
Vanessa Styles	University of Sussex <code>v.styles@sussex.ac.uk</code>	UK
Tor Sørenvik	University of Bergen <code>tor.sorevik@math.uib.no</code>	Norway
Seyyed Hassan Taheri	Ferdowsi University of Mashhad <code>taheri@ferdowsi.um.ac.ir</code>	Iran
Jared Tanner	University of Utah <code>tanner@math.utah.edu</code>	USA
Alan Taylor	University of Strathclyde <code>ta.atay@maths.strath.ac.uk</code>	UK
Petr Tichy	Academy of Sciences of the Czech Republic <code>tichy@cs.cas.cz</code>	Czech Republic
Leonardo Traversoni	Universidad Autonoma Metropolitana <code>ltd@xanum.uam.mx</code>	Mexico
Jan Van lent	University of Bath <code>j.van.lent@maths.bath.ac.uk</code>	UK
Guido Vanden Berghe	Ghent University <code>guido.vandenbergh@UGent.be</code>	Belgium
Heinrich Voss	Hamburg University of Technology <code>voss@tuhh.de</code>	Germany
Jerzy Wasniewski	Danish Technical University <code>jw@imm.dtu.dk</code>	Denmark
Andy Wathen	Oxford University <code>wathen@comlab.ox.ac.uk</code>	UK
Alistair Watson	Dundee University <code>gawatson@maths.dundee.ac.uk</code>	UK
Andre Weideman	University of Stellenbosch <code>weideman@sun.ac.za</code>	South Africa
Richard Welford	University of Sussex <code>r.r.welford@susx.ac.uk</code>	UK
Sohrab Ali Yousefi	Shahid Beheshti University <code>s-yousefi@cc.sbu.ac.ir</code>	Iran
Gaetano Zanghirati	University of Ferrara <code>g.zanghirati@unife.it</code>	Italy

Abstracts of Invited Talks

Piecewise polynomial differential forms and mixed finite elements

Douglas Arnold & Richard Falk, Ragnar Winther
(*University of Minnesota*)

The finite element exterior calculus reveals the relationship between and unity among many different families of finite elements. It allows for a better understanding of their properties, and new ideas for their implementation. In particular, it reveals the special role of two families of finite element spaces for $H(\text{curl})$ and $H(\text{div})$, which are distinct but inter-related generalizations of standard Lagrange family of finite elements for H^1 . These space can be constructed in a uniform, dimension-independent way using the Koszul complex. They can be combined in a variety of ways into finite dimensional subcomplexes of the de Rham complex which can be related to the de Rham complex via bounded projections which commute with exterior differentiation. From this structure follow the stability properties which make these elements effective in practice for solving a variety of partial differential equations. In addition we will discuss the construction of natural geometric bases for all the spaces, which generalize the Bernstein basis for Lagrange elements.

Numerical analysis of a nonlocal integro-differential equation

Dugald Duncan & Samir Bhowmick (*Heriot-Watt University*)

The integro-differential equation (IDE)

$$u_t = \varepsilon \int_{\Omega} J(x-y)(u(y,t) - u(x,t))dy + f(u)$$

with symmetric kernel $J \geq 0$ and bistable $f(u)$ (e.g., $f(u) = u - u^3$), has been proposed as a model of phase separation. This and similar IDEs appear in combination with other equations in more complicated phase separation models, as well as in diverse models of population dynamics and even in neuroscience

Models of this type have roots in the work of Van der Waals (1893), dealing with equilibrium of liquid and gas in a capillary tube. In that paper he essentially used a nonlocal formulation, but finally Taylor expanded and truncated it to derive a PDE. For example, in the IDE above, Taylor expansion of $u(y,t)$ about $y = x$ and some rough approximation leads to the Allen-Cahn PDE

$$u_t = \mu \Delta u + f(u),$$

where $\mu \propto \varepsilon$. Despite the formal connection, the behaviour of solutions of the IDE and Allen-Cahn equation are different in important aspects.

In general one can only successfully approximate (or replace) such IDEs by PDEs in special cases, and so the IDE models deserve attention themselves. This talk concentrates on the numerical approximation of the IDE above, and highlights properties that can be exploited to obtain results surprisingly efficiently.

Separating clusters of points and training SVMs

Roger Fletcher & Gaetano Zanghirati (*University of Dundee*)

Finding the hyperplane that best separates two clusters of points is an important problem in many areas, and particularly in training Support Vector Machines (SVMs). The desirable solution is shown to satisfy an NLP problem with a single nonlinear constraint. Existing methodology transforms this problem to a dual convex QP problem, but is shown to be unreliable in many situations. A new proposal based on the SQP method is described, along with numerical experience. Potential applications can have a very large number of points in the clusters and are computationally challenging. We outline an approximation scheme based on low-rank Cholesky factors.

Radial Basis Functions for Solving PDEs - Some Recent Developments

Bengt Fornberg (*University of Colorado*)

Radial basis functions (RBFs) originated in the 1970s as a method for interpolating scattered data. More recently, both our knowledge about RBFs and their range of applications have grown tremendously. They easily generalize to multiple dimensions, handle irregular domains, and can be spectrally accurate both for interpolation and for solving PDEs. We will discuss some key properties of RBF interpolants and also a couple of computational algorithms for RBFs which bypass ill-conditioning issues in the particularly interesting case of relatively flat basis functions. The standard way to numerically implement RBFs is merely a potentially ill-conditioned algorithm for a genuinely well-conditioned problem. These algorithms can be very advantageous when using RBFs to solve PDEs.

Ten ways to compose a tensor

Gene Golub & Lek-Heng Lim (*Stanford University*)

In scientific and statistical computing, one often reduces the problem at hand – be it a problem involving differential equations or nonlinear optimization or parameter estimation – to a simpler problem (or a sequence of these) that requires nothing more than linear algebra. In fact, the solution of linear systems is of fundamental importance in supercomputing and underlies many scientific computations. However, with the use of increasingly sophisticated sensor devices, experimental methodologies, and mathematical models, we now see a new generation of problems in scientific and statistical computing that cannot be reduced to standard problems in numerical linear algebra. It is thus pertinent to enlarge the arsenal of computational tools available at our disposal. Among the various plausible extensions to numerical linear algebra, one will find the capability of dealing with multilinearity to be among the most natural, desirable, and powerful – if we could do tensor computations (numerical multilinear algebra) as effectively as matrix computations (numerical linear algebra), then we would be able to address many of the new problems arising in modern scientific and statistical computing.

It is not coincidental that “the decompositional approach to matrix computations” has been named one of the Top 10 Algorithms of the 20th Century. If numerical linear algebra is the foundation of scientific computing, then matrix decompositions may be considered to be the foundation of numerical linear algebra. So the development of numerical multilinear algebra ought to begin with a few basic tensor decompositions.

In this talk, we will present ten decompositions of tensors and discuss their properties and applications. Our list will include the tensorial generalizations of LU/LDU decomposition, QR/complete orthogonal factorization, eigenvalue decomposition (EVD), singular value decomposition (SVD), non-negative matrix factorization (NMF), Kronecker product decomposition, and more. We will discuss the similarities and differences of these decompositions with their matrix counterparts, as well as the various challenges in numerical multilinear algebra, of which these tensor decompositions form a cornerstone.

To every tensor decomposition, there is an associated approximation problem. We will see how these may be applied to multilinear statistical models that generalize vector space models, independent component analysis, graphical models/Bayesian networks, and model reduction. We

will illustrate these with selected applications in bioinformatics, computer vision, signal processing, spectroscopy, and sensor location.

hp-Adaptive Discontinuous Galerkin FEMs on Isotropic and Anisotropically Refined Meshes

Paul Houston (*University of Nottingham*)

We present an overview of some recent developments concerning the *a posteriori* error analysis and adaptive mesh refinement of non-conforming discontinuous Galerkin (DG) finite element methods for the numerical solution of second-order PDEs with non-negative characteristic form. Here, we shall be particularly concerned with the derivation of *a posteriori* bounds on the error measured in terms of certain output functionals of the solution of practical interest; relevant examples include the lift and drag coefficients for a body immersed into a fluid, the local mean value of the field or its flux through the outflow boundary of the computational domain, and the pointwise evaluation of a component of the solution.

By employing a duality argument we derive so-called weighted or Type I *a posteriori* estimates which bound the error between the true value of the prescribed functional, and the actual computed value. In these error estimates, the element residuals of the computed numerical solution are multiplied by local weights involving the solution of a certain *dual* or *adjoint* problem. On the basis of the resulting *a posteriori* error bound, we design and implement an *hp*-adaptive finite element algorithm to ensure reliable and efficient control of the error in the computed functional with respect to a user-defined tolerance. Here, the adaptive algorithm employed will be based on a combination of local isotropic and anisotropic refinement of the computational mesh and local polynomial degrees. Numerical experiments highlighting the performance of the proposed anisotropic *hp*-adaptive strategy will be presented.

This research has been carried out in collaboration with Edward Hall (University of Nottingham) and Manolis Georgoulis (University of Leicester).

Wavelet Methods for PDE-Constrained Control Problems: Optimal Preconditioners, Fast Iterative Solvers, and Adaptivity

Angela Kuno (*University of Bonn*)

The numerical solution of PDE-constrained control problems requires to repeatedly solve a system of PDEs for the involved variables (state, costate and control). Considering specifically constraints in form of a linear elliptic PDE, we aim at deriving

most efficient numerical solution schemes. These schemes will be based on wavelet representations which yield uniformly bounded condition numbers of the system matrices and which, together with nested iteration, provide fast solution schemes of optimal linear complexity on uniform discretizations. A further substantial reduction of complexity can be achieved by introducing adaptivity for solutions exhibiting singularities. For discretizations based on wavelets, we are able to prove convergence of an adaptive scheme together with optimal complexity estimates when compared to the wavelet-best N -term approximation.

Finally, I would like to address PDE-constrained control problems with additional inequality constraints on the control which pose substantial difficulties for deriving fast numerical solution schemes.

A New Perspective on the Lattice Boltzmann Method for Simulating Fluid Flow

Jeremy Levesley & Robert Brownlee and Alexander Gorban (*University of Leicester*)

The Navier-Stokes' equations are the main model of choice for fluid flow. The Lattice Boltzmann Method (LBM) for simulating fluid flow starts from the kinetic equation

$$\frac{Df}{Dt} = J(f),$$

where f is the distribution function in phase space, and J represents some sort of collision process. Macroscopic variables are recovered by integration of the distribution function against low degree polynomials of the velocity. LBM is a discrete version of this process.

We will show that the LBM should be viewed as a free-flight in phase space followed by a equilibration process, which does not change mass, momentum and energy densities and deals properly with the entropy in the system. We show that the Navier-Stokes' equations are reproduced via this process, up to second order in the free-flight time τ (which is a computational parameter).

In addition to this we will show how a new LBM algorithm, involving a 'magic step' stabilises the conventional LBM and allows us to use multispeed lattices with a consequent increase in the possibility for thermal simulation.

The Return of the Filter

Sven Leyffer & Roger Fletcher (*Argonne National Laboratory*)

Filters have been introduced as an alternative to penalty functions to promote global convergence

for nonlinear optimization algorithms. A filter borrows ideas from multi-objective optimization and accepts a trial point whenever the objective or the constraint violation is improved compared to previous iterates.

We present recent developments in filter methods. We review new active set approaches to nonlinear optimization based on a two-phase methodology. The first finds an estimate of the optimal active set, and the second phase performs a Newton step on the corresponding equality constrained problem. We present recent ideas that allow inexact subsystem solves. Time permitting we present recent numerical experience with a range of filter methods, including a novel non-monotone filter method.

Numerical solution of optimal control problems for differential-algebraic systems

Volker Mehrmann & Peter Kunkel (*Technische Universität Berlin*)

Optimal control problems for differential-algebraic systems (descriptor systems) arise in many applications ranging from flow control to multi-body dynamics. We discuss optimal control problems for general unstructured nonlinear differential-algebraic equations of arbitrary index. We derive necessary conditions in the case of linear-quadratic control problems and extend them to the general nonlinear case. Moreover, we discuss the numerical solution of the resulting two-point boundary value problems and present a numerical example.

Stochastic Finite Elements and Fast Iterative Solvers

David Silvester (*University of Manchester*)

Simulation of the motion of an incompressible fluid and the transport of chemicals in porous media is a very challenging problem. In deterministic groundwater flow modelling, inputs such as material properties, boundary conditions and source terms are assumed to be known exactly. The so-called Stochastic Finite Element Method provides a framework for incorporating statistical information about spatial variability in material parameters so that more comprehensive information about the flow can be obtained. Instead of performing multiple deterministic simulations, one large calculation is performed incorporating assumed statistics of the random inputs. The output can be post-processed to determine probabilistic information such as the expected concentration of a chemical in the groundwater at a nuclear waste storage site.

This methodology will be reviewed in the talk with a particular focus on computational efficiency. If

stochastic finite element methods are to be competitive with traditional deterministic methodologies based on multiple realisations then we need fast and robust linear algebra techniques to solve the large indefinite systems that arise. We describe a generic block preconditioning technique for such systems with the property that the eigenvalues of the preconditioned matrices are contained in intervals that are bounded independently of the mesh size. An attractive feature is that the basis of the preconditioning is a readily available building block; namely, a scalar diffusion solve based on an algebraic multigrid V-cycle.

This is ongoing work with Oliver Ernst and Elisabeth Ullmann from Freiberg and with Catherine Powell from the University of Manchester. It is supported by the DAAD and British Council under ARC collaborative project grant 1279.

On unexpected consequences of numerical stability analysis of Krylov subspace methods

Zdenek Strakos & Dianne P. O’Leary, Petr Tichý and Chris C. Paige (*Academy of Sciences of the Czech Republic*)

Until recently, rounding error analysis for iterative methods for solving large linear algebraic systems, and for Krylov subspace methods in particular, was considered not well developed. [Higham, N.J., *Accuracy and Stability of Numerical Algorithms*, SIAM, Philadelphia, 2002, Section 17] gives two main reasons. First, in many applications accuracy requirements are modest and can be satisfied without difficulty. Second, rounding error analysis for iterative methods is inherently more difficult than for direct methods, and the results are harder to interpret.

Within the last decade, an interest in rounding errors analysis for Krylov subspace methods has, however, considerably increased. It was observed that rounding errors can delay convergence and significantly increase the cost of computation even *when stopping at a modest accuracy level*. The delay phenomenon in the conjugate gradient method (CG) was linked to the finite precision behaviour of the Lanczos method, and it was understood. Estimates of the energy norm of the error in CG were justified by a mathematically rigorous rounding error analysis. Results on limiting accuracy of various methods gave a guidance for their implementations. On the other hand, rounding error analysis for seemingly attractive implementations used in practice revealed their hidden potentially dangerous numerical instabilities.

In our contribution we illustrate on two recent de-

velopments that rounding error analysis can have a surprising impact in other areas of research. In the first part we show that Gauss-Christoffel quadrature for a small number of quadrature nodes can be highly sensitive to small changes in the distribution function, and we describe the relationship of the sensitivity of Gauss-Christoffel quadrature to the convergence properties of the CG and Lanczos methods in finite precision arithmetic. In the second part we explain how rounding error analysis of the generalized minimal residual method (GMRES) has resulted in the core problem decomposition of orthogonally invariant linear algebraic approximation problems. In both cases, rounding error analysis for an iterative method has inspired questions in the areas far from the original problem. Their solution has offered a new insight to mathematical foundations of the classical problems.

New perspectives for stochastic simulations: mathematical and numerical issues.

Denis Talay (*INRIA*)

The objective of the lecture is to present recent mathematical and numerical results and open questions on stochastic numerical methods for parabolic or elliptic problems, linear or nonlinear, especially when the equations include singularities. We will also describe applications in Finance, Biology, and Meteorology.

Contributed Abstracts

Experience with Gradient Methods Based on Self-Scaling Quasi-Newton Updates

Mehiddin Al-Baali (*Sultan Qaboos University*)

Some modified Barzilai-Borwein gradient methods for solving large-scale quadratic optimization problems will be considered. A new approach for the Barzilai-Borwein method and new modified methods will be derived on the basis of self-scaling quasi-Newton updates. Numerical experiments will be described.

GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting

Mario Arioli & Iain S. Duff, Serge Gratton, and Stephane Pralet (*Rutherford Appleton Laboratory*)

A strict adherence to threshold pivoting in the direct solution of symmetric indefinite problems can result in substantially more work and storage than forecast by an sparse analysis of the symmetric problem. One way of avoiding this is to use static pivoting where the data structures and pivoting sequence generated by the analysis are respected and pivots that would otherwise be very small are replaced by a user defined quantity. This can give a stable factorization but of a perturbed matrix.

The conventional way of solving the sparse linear system is then to use iterative refinement (IR) but there are cases where this fails to converge. We will discuss the use of more robust iterative methods, namely GMRES and its variant FGMRES and their backward stability when the preconditioning is performed by HSL_M57 with a static pivot option.

References

[1] Arioli M., Duff I. S., Gratton S., and Pralet S., 2006. A note on GMRES preconditioned by a perturbed LDL^T decomposition with static pivoting. RAL-TR-2006-007

A MATLAB Tool-kit for 3D Cone Beam Computerised Tomography

Dhavid Aruliah & K. Jackson, D. Moseley, N. Rezvani, and J. Siewerdsen. (*University of Ontario Institute of Technology*)

Advances in x-ray detectors within the last ten years has improved the quality of computerised tomography (CT) volumetric imaging systems significantly. In particular, data acquisition using high resolution flat-panel x-ray detectors permits cone-beam computerised tomography (CBCT). Earlier

technologies relied on acquiring a large number of scans of horizontal slices using parallel- or fan-beam geometries and performing two-dimensional reconstructions over each slice. CBCT systems capitalise on rapid acquisition of circular cone-beam data in a single scan and subsequently use the Feldkamp-Davis-Kress (FDK) formulation for three-dimensional reconstructions. We summarise some of existing CT methods and present some of our Matlab implementation that bundles FDK-type schemes with the intention of providing an open-source research tool.

A Fast Multigrid Algorithm for the Chan-Vese Image Segmentation Model in Variational Formulation

Noor Badshah & Ke Chen (*University of Liverpool*)

Variational models based on nonlinear optimisation and nonlinear partial differential equations are increasingly used to complement traditionally linear techniques widely used in image processing communities.

This paper will be concerned about image segmentation, which is a fundamental task in many applications including MRI techniques. The Chan-Vese model [1] of active contours without edges computes the segmented image $u = c_1 H(\phi(x, y)) + c_2(1 - H(\phi(x, y)))$ from

$$\min_{\phi, c_1, c_2} F(\phi, c_1, c_2)$$

where

$$\begin{aligned} F(\phi, c_1, c_2) = & \mu \int_{\Omega} \delta(\phi) |\nabla \phi| dx dy \\ & + \lambda_1 \int_{\Omega} |z(x, y) - c_1|^2 H(\phi) dx dy \\ & + \lambda_2 \int_{\Omega} |z(x, y) - c_2|^2 (1 - H(\phi)) dx dy \end{aligned}$$

and has been used successfully for segmentation of images. Here z is the given image with many features, ϕ is a level set function whose zero contour Γ is of interest, c_1, c_2 are the average values of image inside and outside Γ and H, δ are Heaviside and Dirac delta functions respectively. The Euler-Lagrange solution resulting from minimization of the above energy is a fully nonlinear partial differential equation. The model is usually solved by using time marching methods (involving artificial time step) with semi-implicit schemes. The recent method of Additive Operator Splitting (AOS) provides an effective acceleration of such schemes for images up to moderate sizes. However to process images of large size, urgent need exists in developing fast multilevel methods.

This paper presents a multigrid method to solve the Chan-Vese partial differential equation independent of artificial time step, and demonstrates its fast convergence. Some analysis is presented to justify the associated smoothers employed. A surprising finding is that our nonlinear multigrid method, apart from fast convergence, is more likely to converge to the global minimizer of the particular non-convex minimisation problem than previously used unilevel methods which may get stuck at local minimizers. Finally our results are compared to a new model [2] which aimed to resolve the global minimisation issue of [1].

[1] T. F. Chan and L. A. Vese, "Active contours without edges", *IEEE Trans. Image Proc.*, 10(2):266-277, 2001.

[2] T. F. Chan, S. Esedoglu and M. Nikolova, "Algorithm for finding global minimizers of image segmentation and de-noising models", *SIAM J. Appl. Math.*, 66 (5):1632-1648, 2006.

Moving mesh methods for time-dependent PDEs which evolve best L_2 fits.

Mike Baines (*University of Reading*)

Moving mesh discretizations of (possibly moving) boundary value problems governed by time dependent scale-invariant PDEs are presented, in which the mesh is moved so as to conserve a (weak) integral.

It is shown that for a class of such problems which conserve mass, self-similar solutions and L_2 best fits to self-similar solutions are evolved exactly in time.

Schemes are constructed which approximately possess these properties in the event of self-similar initial data.

Coupled vehicle-skin models for drug release

Silvia Barbeiro & J.A. Ferreira (*University of Coimbra*)

We propose mathematical models for percutaneous drug absorption. The diffusion processes of finite doses of a drug through the vehicle and through the skin are considered. The new models are established introducing in the classical Fick's law a memory term being the diffusion equations of the classical models replaced by integro-differential equations. The stability analysis of the resulting models is carried out. Methods for the computation of numerical solutions are proposed. Stability and convergence of the introduced methods are studied. Finally, numerical simulations illustrating the behavior of the models are included.

A formula for the error of finite sinc-interpolation with an even number of nodes

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

Recently we gave a formula for the error committed when truncating the sinc-series of a function that does not decrease sufficiently rapidly for the discarded tails of the series to be negligible. The main part of the formula is a polynomial in the distance between the nodes whose coefficients contain derivatives of the function at the extremities.

The middle term of a sinc-series usually corresponds to the origin, so that its symmetric truncation contains an odd number of terms, one for every node.

In our talk we give the formula for the case of an even number of nodes. We hope to give also some applications of the formulas.

Particular and Fundamental Solution Methods for Scattering Problems

Timo Betcke (*The University of Manchester*)

Methods based on particular and fundamental solutions are an accurate tool to solve Laplace eigenvalue and Helmholtz boundary value problems. The idea is to approximate the solution from a space of functions that already satisfy the Helmholtz equation but not necessarily the boundary conditions.

In this talk we extend these ideas to exterior scattering problems. We discuss the properties of different basis sets that already satisfy the Sommerfeld radiation condition and propose a domain decomposition approach for domains with corners that combines Fourier-Bessel functions to capture the corner singularities and Hankel functions to satisfy the Sommerfeld radiation condition.

Minmax principle for magnetic stationary Schrödinger equation

Marta Betcke & Heinrich Voss (*University of Manchester*)

In this contribution we consider the Zeeman splitting of energy levels of quantum dots and rings in a homogenous magnetic field. Quantum dots are semiconductor nanostructures in which the free carriers are confined by the potential barriers to a small region in all three directions of space. Moreover, if the size of the region is smaller than an electron wavelength the energy states become quantized at discrete energy levels as it happens in an atom. This property makes the quantum dots very attractive for applications in micro and optoelectronic devices and allows to use them for investigating systems at the atomic level.

We derive a pair/quadruple of nonlinear eigenvalue problems corresponding to the one-band effective Hamiltonian governing the electronic states of a quantum dot/ring in a homogenous magnetic field. We show, that the pair/quadruple of nonlinear problems allows for the minmax characterization of its eigenvalues under certain conditions, which are satisfied for our examples and the common InAs/GaAs heterojunction. Exploiting the minmax property we devise efficient iterative projection methods simultaneously handling the pair/quadruple of nonlinear problems and thereby saving about 25%/30–40% of the computation time comparing to the Nonlinear Arnoldi method applied to each of the problems separately.

Mathematical and Numerical Modelling of Cellular Cholesterol Homeostasis

Bonhi Bhattacharya & Anne-Marie Minihane, Peter Sweby (*University of Reading*)

Elevated plasma cholesterol levels are a major risk factor for the development of coronary heart disease. The level of circulating cholesterol in the blood stream is determined by dietary intake and its rate of production in the body, and by its rate of removal from the blood stream.

The major route of cholesterol removal from the circulation is via uptake by the liver. Intracellular cholesterol concentration in liver cells is regulated by mechanisms which function overall to maintain cholesterol levels at the optimum value for the cell. This occurs via a combination of feedback inhibition modulation of pathways of internal cholesterol biosynthesis, and influx and efflux of cholesterol to and from the liver cell. This mechanism of homeostasis ultimately governs the rate of hepatic cholesterol uptake from the plasma.

We present the initial development of a mathematical model of cellular cholesterol homeostasis, focussing on pathways of cholesterol biosynthesis and utilisation, which is used to investigate dynamical properties of feedback inhibition models. The model is a nonlinear system of ODEs, containing experimental parameters, derived from mass action modelling of the reaction pathways. Preliminary numerical results will be presented.

The Solution of 2D Unsteady Navier-Stokes Equations using Boundary Element Method with Time-dependent Fundamental Solution

Nuray Bozkaya (*Middle East Technical University*)

The two dimensional unsteady, laminar flow equations of an incompressible viscous fluid are solved

by using the boundary element method (BEM). The flow equations are taken in terms of stream function and vorticity and solved iteratively. The stream function equation is solved by using the dual reciprocity boundary element method (DRBEM), whereas in the vorticity equation the BEM is used with the time-dependent fundamental solution. The integrals, over the time intervals and space elements, appearing in the entries of the element matrices are computed numerically.

Constant boundary elements are used in the discretization of the space domain. Since the BEM is applied directly to the vorticity transport equation with the corresponding time-dependent fundamental solution, the necessity of using another time integration scheme is eliminated. The numerical results are presented for some test problems and for small values of Reynolds number.

A coupled differential quadrature time integration scheme with dual reciprocity boundary element method applied to the unsteady Navier-Stokes equations

Canan Bozkaya (*Middle East Technical University*)

The 2-D time dependent Navier-Stokes equations in terms of the vorticity and the stream function are solved numerically by using the coupling of the dual reciprocity boundary element method (DRBEM) in space with the differential quadrature method in time. The DRBEM enables us to use the fundamental solution of Laplace's equation, which is easy to implement computationally. The convective terms in the vorticity transport equation are considered as the nonhomogeneity in the equation and are approximated by radial basis functions.

The solution of the Poisson equation which links stream function and vorticity with an initial vorticity guess produces velocity components in turn for the solution of the vorticity transport equation. The DRBEM formulation of the vorticity transport equation results in an initial value problem represented by a system of first order ordinary differential equations in time. When the DQM discretizes this system in time direction, we obtain a system of linear algebraic equations which gives the solution vector for vorticity at any required time levels without the use of an iterative scheme in time. The procedure outlined here is applied to some test problems including the lid-driven cavity problem. The numerical results are visualized in terms of stream function and vorticity contours for several values of Reynold's number (Re) ranging from $Re = 1$ to $Re = 1000$.

Multiple solutions of systems of nonlinear algebraic equations and their connection with the matrix polynomial theory

Mikhail Bulatov & Chistyakov V.F. (*Institute of System Dynamics and Control Theory of Siberian Branch of Russian Academy of Sciences*)

Consider the system of non-linear algebraic equations

$$F(x) = 0, \quad F : R^n \rightarrow R^n.$$

If $x^* : F(x^*) = 0$ and $\det \partial F / \partial x|_{x=x^*} = 0$ then such a solution is said to be multiple. We put a matrix polynomial into correspondence with the initial system and give the definition of multiplicity of solution x^* in terms of matrix index. This definition coincides with the classic definition of multiplicity when $n = 1$.

Using different examples, we show the connection between the notation of multiplicity, introduced in algebraic geometry, and the definition of multiplicity proposed by the authors. It is demonstrated how the announced results can be applied to analyzing critical points (maximum, minimum) and DAEs with multiple solution. Problems of convergence for the Newton method with respect to multiplicity are discussed.

The work has been supported by Russian Foundation For Basic Research (project No. 07-01-9000, project No. 06-01-81013) and project No. 5 SB RAS.

An Adaptive Finite Element Approximation of the Ambrosio-Tortorelli Functional

Siobhan Burke & Christoph Ortner, Endre Süli (*Oxford University*)

A model for brittle fracture, proposed by Francfort and Marigo (1998), is formulated in terms of minimizing a highly irregular energy functional. One method for working with this model numerically is to use the Ambrosio – Tortorelli functional, which approximates the Francfort – Marigo functional in the sense of Gamma convergence. The problem is then reduced to minimizing an elliptic functional of two variables, which is convex and coercive in each. By alternately minimizing over each variable, a finite element method can be used to construct approximations to local minimizers of the Ambrosio-Tortorelli functional. In this talk I will present a residual based adaptive finite element algorithm for their efficient computation.

A new perspective on the complexity of interior point methods for linear programming

Coralia Cartis & Raphael Hauser (*Rutherford Appleton Laboratory*)

In a dynamical systems paradigm, many optimization algorithms are equivalent to applying forward Euler method to the system of ordinary differential equations defined by the vector field of the search directions. Thus the stiffness of such vector fields will play an essential role in the complexity of these methods. We first exemplify this point with a theoretical result for general linesearch methods for unconstrained optimization, which we further employ to investigating the complexity of a primal short-step path-following interior point method for linear programming. Our analysis involves showing that the Newton vector field associated to the primal logarithmic barrier is nonstiff in a sufficiently small and shrinking neighbourhood of its minimizer. Thus, by confining the iterates to these neighbourhoods of the primal central path, our algorithm has a nonstiff vector field of search directions, and we can give a worst-case bound on its iteration complexity. Furthermore, due to the generality of our vector field setting, we can perform a similar (global) iteration complexity analysis when the Newton direction of the interior point method is computed only approximately (using some direct method for solving linear systems of equations). Also, if we choose a particular rescaling of the Newton direction as our nonstiff vector field, we show that the interior point method of our analysis has polynomial worst-case iteration complexity.

A robust r-adaptive method for a singularly perturbed 1d reaction-diffusion problem

Naresh Chadha & Natalia Kopteva (*University of Limerick*)

We present a robust r -adaptive method for a singularly perturbed reaction-diffusion two point boundary problem, whose solutions typically exhibit sharp boundary layers. The method used is adaptive movement of mesh points by equidistribution of a suitable monitor function, which is based on the maximum norm a posteriori error estimates of [1]. We investigate the fully discretized problem, extending the analysis [2] to a new problem and a new monitor function. We state general sufficient conditions for the existence of a solution of an equidistribution problem involving an arbitrary discrete operator and an arbitrary monitor function. Furthermore, it is shown that starting from a uniform mesh, the algorithm used provides a mesh on which our computed solution is second-order ε -uniformly accurate. The number of steps taken by the algorithm to achieve this accuracy is estimated to be of order $O(\ln(1/\varepsilon)/\ln N)$. We conclude by presenting supporting numerical results and an overview of our future work. [1] N. Kopteva,

Maximum norm of a posteriori error estimates for a one-dimensional singularly perturbed semilinear reaction-diffusion problem, *IMA Journal of Numer. Anal.*, (2005) [2] N. Kopteva and M. Stynes, A robust adaptive method for a quasilinear one dimensional convection-diffusion problem, *SIAM J. Numer. Anal.* 39 (2001) 1446-1467.

Asymptotic Stability of a Jump-SDE and its Numerical Approximation

Graeme Chalmers & D. J. Higham (*University of Strathclyde*)

Stability is an important property in any timestepping scenario. For stochastic differential equations (SDEs), two very natural, but distinct, concepts are mean-square and asymptotic stability. Mean-square stability is more amenable to analysis, and hence this property dominates in the literature. Asymptotic stability has received some attention in the case of non-jump SDEs. However, in the jump-SDE context, which is becoming increasingly important in mathematical finance, we are only aware of mean-square results. This provides motivation for the study of asymptotic stability in the jump-SDE setting.

We consider a natural extension of the classical linear ODE test problem that includes both diffusion and jump components. Asymptotic stability of the problem is characterised in terms of its four parameters, and a corresponding stability condition for a theta-method discretisation is derived.

One interesting observation is that a backward Euler method does not give uniformly better stability than a forward Euler version. Furthermore, although the stability condition for the theta-method is analytically intractable, we are able to prove that these methods always preserve stability/instability for sufficiently small timesteps.

Pseudospectra of Matrix Polynomials expressed in alternative bases

Rob Corless & Amir Amiraslani and Nargol Rezvani (*University of Western Ontario*)

Spectra and pseudospectra of matrix polynomials are of interest in geometric intersection problems, vibration problems, and analysis of dynamical systems. In this note we consider the effect of the choice of polynomial basis on the pseudospectrum and on the conditioning of the spectrum of regular matrix polynomials. In particular, we consider the direct use of the Lagrange basis on distinct interpolation nodes, and give a geometric characterization of “good” nodes. We also give some tools for computation of roots at infinity via a new, natural, reversal. The principal achievement of the paper is to

connect pseudospectra to the well-established theory of Lebesgue functions and Lebesgue constants, by separating the influence of the scalar basis from the natural scale of the matrix polynomial, which allows many results from interpolation theory to be applied.

A posteriori error estimates for time discretizations of fully non-linear parabolic problems in Banach spaces

Eduardo Cuesta & Ch. Makridakis (*University of Valladolid*)

In this paper we consider a time discretization of an abstract fully non-linear parabolic problem

$$u' = F(u), \quad t \geq 0, \quad u(0) = u_0,$$

where $F : X \rightarrow X$ is a differentiable map, X is a complex Banach space and $u_0 \in X$.

Our contribution consists in obtaining a posteriori error estimates of conditional type, i.e. are valid under assumptions solely on the numerical solution, for such a discretizations in the abstract setting of the complex Banach spaces X . In fact, the numerical method considered is the backward Euler method and the proofs are based on suitable fixed point arguments fitting in the maximal regularity framework of Banach spaces.

Discontinuous Galerkin approximations for first kind Volterra integral equations

Penny Davies & Hermann Brunner, Dugald B Duncan (*University of Strathclyde*)

We present new convergence results for piecewise polynomial discontinuous Galerkin (DG) approximations of a first kind Volterra integral equation of convolution kernel type, where the kernel K is smooth and satisfies $K(0) > 0$. We show that a m -th degree DG approximation exhibits global convergence of order m when m is odd and order $m+1$ when m is even. There is local superconvergence of one order higher (i.e. order $m+1$ when m is odd and $m+2$ when m is even), but in the even order case there is superconvergence only if the exact solution u of the equation satisfies $u^{(m+1)}(0) = 0$. We also present numerical test results which show that these theoretical convergence rates are optimal.

Numerical Differentiation on Scattered Centres

Oleg Davydov (*University of Strathclyde*)

We discuss algorithms for numerical differentiation based on local data fitting on scattered centres. Error bounds, numerical examples and applications to

certain meshless methods of discretisation of PDEs will be presented.

The smallest deviation from consistency

Achiya Dax (*Hydrological Service*)

The need for solving a system of linear inequalities, $Ax \geq b$, arises in many applications. Yet often the system to be solved turns to be inconsistent due to measurement errors in the data vector b . The problem of calculating the smallest correction of b that recovers feasibility is called the least deviation problem. The size of the correcting vector to be minimized is defined by some (arbitrary) norm.

In this talk we present new results about the geometry and the duality features of this problem, which are quite different from those of the related linear least norm problem. For example, the set of all the points f for which the linear system $Ax \geq f$ is solvable constitutes a closed convex cone, whose polar cone is composed of all the nonnegative vectors that belong to $\text{Null}(A^T)$. Consequently b has a unique polar decomposition into these cones, and the component that belongs to the polar cone provides the smallest correction regarding the Euclidean norm.

It is shown that the dual problem has the following form: maximize $b^T y$ under the restrictions that y belongs to the polar cone, and that the dual norm of y does not exceed 1. Moreover, primal and dual solutions are related by certain "alignment relations". If time allows I will outline an effective affine scaling algorithm for solving the dual problem when using the l_1 norm.

Iterative solution of saddle-point systems with applications from PDE-constrained optimization

Sue Dollar & N. I. M. Gould, W. H. A. Schilders, A. J. Wathen (*Rutherford Appleton Laboratory*)

We will consider that solution of saddle-point problems of the form

$$\underbrace{\begin{bmatrix} H & A^T \\ A & -C \end{bmatrix}}_K x = b,$$

where H is symmetric and C is assumed to be symmetric and positive semi-definite (possibly zero). Such systems arise in a variety of applications. In PDE-constrained optimization problems K often has dimensions of the order 10^6 – 10^9 . When C is positive definite the saddle-point system may be rewritten in 'doubly augmented' form to give an equivalent system which is symmetric and positive definite (Forsgren, Gill and Griffin) thus allowing us to solve the saddle-point system via a conjugate

gradient-style method without the need for a constraint preconditioner.

We will show that this idea can be extended to the case of C being symmetric and positive semi-definite and that the preconditioning step may be carried out by solving a system of the form

$$\underbrace{\begin{bmatrix} G & \tilde{A}^T \\ \tilde{A} & -C \end{bmatrix}}_P z = r,$$

where G is a symmetric and $\tilde{A}$ approximates A in some way. We will call P an inexact constraint preconditioner and show that although K may be highly ill-conditioned, the eigenvalues which determine the convergence of our method will be $\mathcal{O}(1)$ with many clustering around 1, thus resulting in rapid convergence of our iterative method. Our theoretical results will be backed up with numerical examples.

Computational methods for surface PDEs

Charlie Elliott & Gerhard Dziuk (*University of Sussex*)

Partial differential equations on and for evolving surfaces occur in many applications. For example, traditionally they arise naturally in fluid dynamics and materials science and more recently in the mathematics of images. In this talk we describe computational approaches to the formulation and approximation of transport and diffusion of a material quantity on an evolving surface. We also have in mind a surface which not only evolves in the normal direction so as to define the surface evolution but also has a tangential velocity associated with the motion of material points in the surface which advects material quantities such as heat or mass. We describe two approaches:- 1)Evolving Surface Finite Element Method (ESFEM) is based on triangulated surfaces. 2)Eulerian approach based on solving surface PDEs on all level sets of a prescribed level set function which can be done with a mesh independent of the level surfaces.

Numerical Modeling of Flows Subjected to Deforming Boundaries

Hind Fadel (*University of Leeds*)

In this talk, we investigate the accuracy and limitations of a simple numerical model for the simulation of two-dimensional flows in domains whose boundaries are subject to small deformations. In particular, we seek to avoid the use of moving meshes by adopting a fixed mesh and imposing modified boundary conditions at the deforming boundaries.

A finite differences approach is used to approximate this model, formulated in primitive variables.

In order to validate the proposed approach and its performance, we have developed a mixed finite element solver on a moving mesh. This is also based upon a primitive variable formulation, with the mesh updated in an ALE (arbitrary Lagrangian-Eulerian) manner.

The motivation for this work comes from fluid-structure interaction problems, and our interest is in incompressible flows interacting with linear elastic structures. The results presented will initially concern Stokes flow problems; followed by a discussion of the generalization of the models to laminar Navier Stokes equations.

A finite difference method on triangles

Faisal Fairag (*KFUPM*)

This presentation describes a new method for solving Partial Differential Equations (PDE). This method combines the use of features of both Finite Element Methods (FEM) and Finite Difference methods (FDM). Similar to the FEM, this method uses the triangulation technique and function approximation. Moreover, it uses direct discretization of the PDE, similar to the FDM. The basic idea starts by selecting a finite difference representation of the PDE and a triangular element. The selected representation involves nodal point and non-nodal points. Then the selected triangular element is used to approximate the function values of the non-nodal points. This method can be seen as a finite difference method when an irregular nodal arrangement is appropriate for a given problem. Derivation of the method, the solvability of the resulting system, and discussion on error are presented. Several computational examples (Poisson equation and Navier-Stokes equations) with their graphs and tables are also presented.

Direct Search Methods for the Design of PSA Processes

Giovanna Fiandaca & E.S.Fraga, S.Brandani (*UCL, University College London*)

Pressure Swing Adsorption (PSA) is a cyclic separation process which operates between two pressure levels corresponding to adsorption, at high pressure, and solid regeneration or desorption, at low pressure. It has been widely used in industry for gas separation processes (e.g. air separation and H₂ production) as a more economic and effective alternative to other options such as cryogenic, membrane and absorption processes. Recently, PSA has attracted attention as a valuable technology for the

problem of CO₂ capture aimed at addressing global warming due to greenhouse gas emissions.

The aim of our project is the development of computer aided design tools for PSA processes. The focus is on fast cycle operations, needed to reduce capital and operating costs, which poses computational challenges in both modelling and optimisation. The simplest model for a PSA process is based on the assumption of a linear driving force (LDF) to mass transfer between the fluid and the solid adsorbent. It simplifies the model by eliminating the need to describe concentration profiles in the solid. Unfortunately, the LDF model fails to capture the dynamics of fast cycle operations and as a result, we use more detailed diffusion models. These involve coupled nonlinear partial differential and algebraic equations in time and one or two space dimensions. The detailed diffusion models pose challenges for optimisers, especially gradient based methods. As a result, we have investigated the use of direct search methods, such as the Nelder & Mead simplex method, the multidirectional search method and the alternating directions search method.

We will present a summary of the performance of these methods for the design of a PSA process for air separation. The eventual goal is the development of multi-criteria direct search methods for this problem.

Modeling Simple Atmospheric Flows on A Sphere Using Radial Basis Functions

Natasha Flyer & Grady Wright (*National Center for Atmospheric Research*)

Since the early 1990s, radial basis functions (RBFs) have been applied to solve simple elliptical and mixed parabolic partial differential equations (PDEs). Not until 2003 was the RBF methodology applied to spherical geometries, and then only to low algebraic accuracy. The results to be presented are the first study ever to numerically integrate: 1) purely advective PDEs and 2) the full shallow water model on a sphere using RBFs to spectral accuracy. With regard to the former, the two test cases considered are linear advection of a height field over the surface of the sphere and deformational flow that models the spin up of two diametrically opposed vortices. For the shallow water model, only steady-state solutions will be considered. The RBF methodology is evaluated in terms of accuracy and time stability. Comparisons with common spectral methods will be given.

A new approach to recovery on discontinuous Galerkin

Sebastian Franz & Lutz Tobiska, Helena Zarin
(*TU Dresden*)

A new recovery operator $P : Q_n^{disc}(\mathcal{T}) \rightarrow Q_{n+1}^{disc}(\mathcal{M})$ for discontinuous Galerkin is presented. It is based on the idea of projecting the local solution on a given mesh $\mathcal{T}$ into a higher order space on macro mesh $\mathcal{M}$. Therefore we define local degrees of freedom using Legendre polynomials and provide proper linear combinations of them as degrees of freedom on the macro mesh.

We prove

$$Pu = Pu^I$$

(equivalence of projected function and local interpolated function), stability results in several norms and optimal anisotropic error estimates.

In case of bilinear elements we use a supercloseness result by H.-G. Roos and H. Zarin to prove superconvergence of the postprocessed numerical solution.

New preconditioning strategies for eigenvalue problems

Melina Freitag (*University of Bath*)

We propose a way of accelerating two of the most common methods for computing an eigenvector and corresponding eigenvalue of a large sparse non-symmetric matrix, namely inverse iteration and Arnoldi's method. In order to find an eigenvalue near a shift, at each step of these methods a shifted linear system needs to be solved. We use iterative techniques to find the solution to these inner systems. Then we consider preconditioning strategies for inexact inverse iteration and shift-invert Arnoldi's method and show that for eigenvalue problems, a modification of the preconditioner, which we call "tuned" preconditioner has a large impact on the iteration count for the inner solve and hence significantly reduces the total number of inner iterations.

This is joint work with Alastair Spence (University of Bath, UK) and Howard Elman (University of Maryland, USA).

Iterative solution of elliptic control problems with control and state constraints

Emanuele Galligani (*University of Modena and Reggio Emilia*)

This work concerns the solution of optimal control problems by means of nonlinear programming methods. The control problem is formulated into

a finite dimensional nonlinear programming problem by finite difference approximation. An iterative procedure for the solution of this nonlinear program is presented. An extensive numerical analysis of the behaviour of the method is reported on boundary control and distributed control problems with boundary conditions of Dirichlet or Neumann or mixed type.

A modified least-squares FEM with quadrature for nonlinear advection-diffusion-reaction equations

Mahadevan Ganesh & K. Mustapha (*Colorado School of Mines*)

We present, analyze, and implement a modified least-squares fully discrete finite element method (FEM) with quadrature for strongly nonlinear advection-diffusion-reaction equations on smooth and polygonal domains (satisfying a maximum interior angle condition at the corners). The quadrature FEM algorithm and analysis are applicable for a large class of nonlinear functions (including exponentials and polynomials of odd and even degrees) in the unknown variables. In addition, the algorithm requires solutions of only a linear system at each time step, avoiding the expensive Newton iterations. We prove the stability of the modified least-squares solutions by including the effect of the quadrature in computer implementation, and also prove and demonstrate the optimal order convergence of the approximate solutions.

Decoupling temporal and spatial errors in posteriori error estimation for fully discrete nonlinear parabolic problems

Bosco García-Archilla & J. de Frutos and J. Novo (*Universidad de Sevilla*)

Although a posteriori error estimation is nowadays routinely done in the numerical solution of elliptic problems and ordinary differential equations, in the case of partial differential equations of evolution, the topic is much less developed (see e.g., [1], [3], [4] and the references cited therein). One reason is the need to take into account the two kind of errors present: those arising from the spatial discretization, or spatial errors, and those arising from the time integration, or temporal errors. In parabolic or dissipative problems, since the time integration is typically done by an implicit or semi-implicit method, an elliptic problem has to be numerically solved at each time step. Recently [2], it has been noticed that some a posteriori error estimators for elliptic problems correctly estimate the spatial error independently of the size of the temporal errors

presents. In the present work, we provide an explanation of this fact, which we have found to depend on the temporal errors being of the same order in different (Sobolev) norms. We also comment on obtaining error estimates in the above mentioned norms for the BDF formulae when applied to non-linear dissipative equations.

- [1] A. Bergam, C. Bernardi & Z. Mghazli, *A posteriori analysis of the finite element discretization of some parabolic equations*, Math. Comp., **74**, 2005, 1117-1138.
- [2] J. de Frutos, B. García-Archilla and J. Novo *A posteriori error estimates for fully discrete non-linear parabolic problems*, Comput. Methods Appl. Mech. Engrg., (2007), doi:10.1016/j.cma.2007.03.015.
- [3] C. Makridakis & R. H. Nochetto, *Elliptic reconstruction and a posteriori error estimates for parabolic problems*, SIAM J. Numer. Anal., **41**, 2003, 1585-1594.
- [4] T. Stroubulis, I. Babuska & D. K. Datta, *Guaranteed a posteriori error estimation for fully discrete solutions of parabolic problems*, Int. J. Numer. Meth. Engrg, **56**, 2003, 1243-1259.

Inverse-Type Estimates on hp -Finite Element Spaces and Applications

Emmanuil Georgoulis (*University of Leicester*)

This work is concerned with the development of inverse-type inequalities for piecewise polynomial functions and, in particular, functions belonging to hp -finite element spaces. The cases of positive and negative Sobolev norms are considered for both continuous and discontinuous finite element functions. The inequalities are explicit both in the local polynomial degree and the local mesh-size. The assumptions on the hp -finite element spaces are very weak, allowing anisotropic (shape-irregular) elements and varying polynomial degree across elements. Finally, if time permits, the new inverse-type inequalities are applied to derive bounds for the condition number of symmetric stiffness matrices of hp -boundary element method discretisations of integral equations.

Convergence of adaptive FEM for elliptic eigenvalue problems

Stefano Giani & Ivan G. Graham (*University of Bath*)

In this talk we shall present a convergence result for elliptic eigenvalue problems using mesh adaptivity.

The adaptive method we designed uses a marking strategy based on an a posteriori error estimator, together with a second marking strategy devoted to control the oscillations of computed eigenfunctions on the meshes. The convergence result holds under the condition that the starting mesh is fine enough for the particular problem. Also a number of numerical experiments shall be illustrated.

Non-Newtonian Fluids and Finite Elements

Janice Giudice & Endre Süli (*The University of Oxford*)

We will present the equations governing shear-thinning/shear-thickening fluid flow and an adaptive finite element approximation with a-posteriori error bound. Some computational results will be given. An approach to simulating multiple shear-thinning fluids, with different properties, will then be presented with some simple numerical results.

Adaptive cubic over-estimation methods for unconstrained optimization

Nick Gould & Coralia Cartis, Philippe Toint (*Oxford University/RAL*)

Recently Nesterov and Polyak proposed a new globally convergent modification of Newton's method for non-convex unconstrained optimization with an excellent iteration complexity bound. In this talk, we consider the global convergence and complexity of a general class of methods which includes Nesterov and Polyak's proposal, as well as for potentially less expensive variants aimed at the large-scale case. We illustrate our theoretical developments with numerical tests in which it is shown that these new methods are highly competitive with trust-region methods.

DRBEM simulation of natural convection in a square cavity

Sevin Gümgüm (*Izmir University of Economics*)

In this study, the dual reciprocity boundary element method (DRBEM) is applied to solve the natural convection flow in a square cavity. The governing equations are taken in terms of the stream function-vorticity form of the Navier-Stokes equations as well as the energy equation. In the vorticity transport and energy equation the time derivatives are discretized by using finite difference method (FDM) and the solutions are relaxed with suitable parameters. Linear boundary elements and radial basis functions of the type $f = 1 + r$ are made use of in the DRBEM idea.

For obtaining vorticity boundary conditions the stream function equation is discretized on the

boundary by using the Taylor series expansion which permits to use the interior stream function values. The problem being considered here is that of the two-dimensional flow of a Boussinesq fluid of Prandtl number 0.71 in an upright square cavity described in non-dimensional terms by $0 \leq x \leq 1$, $0 \leq y \leq 1$ with y vertically upwards. The solution is presented in terms of streamlines, vorticity contours and isotherms. The results are in very good agreement with the results obtained with other numerical methods.

Incorporating State Space Equality Constraints into Kalman Filtering Methods

Nachi Gupta (*University of Oxford*)

Kalman Filtering is a recursive optimisation algorithm used in tracking problems. Many applications of Kalman Filtering have inherent and known constraints in the physical dynamics of the system that are rarely exploited despite a potentially significant gain. A couple of methods have been proposed as natural extensions to the filter for incorporating state space equality constraints. We will compare two prominent methods and show that under certain conditions, they both result in a mathematically equivalent estimate structure. In applications, the two methods have numerical advantages and disadvantages over one another. We will use a linear and a nonlinear experiment to illustrate these points.

New Quadrature Formulas from Conformal Maps

Nick Hale & L. N. Trefethen (*University of Oxford*)

Gauss-Legendre quadrature is an excellent and widely used tool for integrating analytic functions over finite intervals. However, it has its drawbacks. The nodes are strongly clustered toward the endpoints and the rate of convergence is perhaps not as fast as it could be. I describe how, by use of a conformal map, we obtain a new class of non-polynomial based quadrature methods, which have more evenly spaced nodes and give readily theorems showing improved convergence rates.

Exploiting hyper-sparsity when computing preconditioners for conjugate gradients in interior point m(...)

Julian Hall & Ghussoun Al-Jeiroudi and Jacek Gondzio (*University of Edinburgh*)

When using preconditioned conjugate gradients to solve the augmented system in interior point methods, the preconditioner devised by Al-Jeiroudi,

Gondzio and Hall requires the identification of a full rank square submatrix B of the constraint matrix, analogous to the basis matrix in the revised simplex method. For problems where preconditioned conjugate gradients is a competitive alternative to direct methods, it is critically important that hyper-sparsity is exploited when identifying B . This talk will highlight the huge computational savings that are achieved when hyper-sparsity is exploited and indicate how the techniques can be extended to the more general problem of matrix rank identification.

Relative perturbation results for the singular values/eigenvalues of symmetrically scaled diagonally dominant matrices

Vjeran Hari & Josip Matejas (*University of Zagreb*)

The existing relative perturbation results for the eigenvalues of scaled diagonally dominant Hermitian matrices have been improved and the new relative perturbation bounds for the singular values of symmetrically scaled diagonally dominant square matrices have been derived. In the case of positive or negative definite Hermitian matrices, the new result reduces to the existing one. But in the indefinite case the new bounds are sharper than the existing ones. The result extends to some other classes of scaled diagonally dominant matrices, like skew-Hermitian and “hidden Hermitian” matrices. Using the standard technique with the Wielandt matrix, one easily obtains a new perturbation result for the singular values of symmetrically scaled diagonally dominant matrices. A typical application of these results lies in proving the relative accuracy of the standard Jacobi method when applied to indefinite scaled diagonally dominant Hermitian matrices. It is also used in proving sharp relative accuracy bounds for the Kogbetliantz method which computes the singular value decomposition of triangular or butterfly matrices.

The Canonical Polar Decomposition: Theory and Computation

Nicholas Higham (*University of Manchester*)

The polar decomposition is a well known matrix decomposition that generalizes the polar representation of a complex number. Although few people realise it, two versions of the decomposition are in use and I will explain why the one less frequently seen, which I term the canonical polar decomposition, deserves identifying as a separate entity. I show how the existence and uniqueness of the canonical polar decomposition is readily shown with the aid of the pseudoinverse. I also discuss a new stopping criterion for iterations for computing the unitary polar

factor.

<http://www.maths.manchester.ac.uk/~higham/>

Stability for Stochastic Regime-Switching

Des Higham & Xuerong Mao and Chenggui Yuan
(*University of Strathclyde*)

In some applications a system can undergo an abrupt change, after which new equations of motion become relevant. A very important application area arises in mathematical finance, where, for example, the stock market may lurch between ‘confident’ and ‘nervous’. This effect can be modelled using a stochastic differential equation where one parameter, the volatility, is allowed to switch between two different levels according to an independent Markov chain. Generally, simulating such a regime-switching (or Markov-switching) system is not much harder than simulating a standard stochastic differential equation. However, existence, uniqueness, numerical convergence and stability theories are yet to be fully worked out. I will give an overview of some mean-square stability results for discretisations based on the theta method.

Analysis of the total least squares problem with multiple right-hand sides

Iveta Hnetynkova & M. Plesinger, Z. Strakos
(*Institute of Computer Science, Academy of Sciences of the Czech Republic*)

In collaboration with D. Sima, S. Van Huffel.

Let A be a real m by n matrix and b a real vector of the length m . In *C. C. Paige, Z. Strakoš: “Core problems in linear algebraic systems”, SIAM J. Matrix Anal. Appl. 27, pp. 861–875 (2006)*, it is proved that for any orthogonally invariant linear approximation problem $Ax \approx b$, the partial Golub-Kahan bidiagonalization of the matrix $[b, A]$ determines a minimally dimensioned *core approximation problem* $A_{11}x_1 \approx b_1$ containing the necessary and sufficient information for solving the original problem. It is shown how the core problem can be used in a simple and efficient way for solving the total least squares and the data least squares formulation of the original approximation problem.

In this contribution we concentrate on a possible generalization of the core problem idea to total least squares problems $AX \approx B$ with *multiple right-hand sides*. Here the existence of $d > 1$ simultaneously approximated columns of the matrix B can lead to significant complications. We investigate a reduction of the original data, and solvability of the resulting reduced problem. Difficulties with the definition of the solution in the total least squares formulation will be illustrated on examples.

A Moving Mesh Finite Element Approach to Phase Change Problems

Matthew Hubbard & M J Baines, P K Jimack and R Mahmood (*University of Leeds*)

The application of the moving mesh finite element method of Baines, Hubbard and Jimack [1, 2] to one- and two-phase Stefan problems will be presented. The method was developed for the simulation of multidimensional free and moving boundary problems and is novel in that it uses the underlying partial differential equation to determine mesh node velocities, both internally and on the moving boundary, rather than the dependent variables (as is more usual). These are instead recovered from a local conservation principle.

A modified version of the original approach will be presented which (a) solves for the rate of change of the conserved quantity (chosen here to represent the “mass” associated with the system) at the same time as the mesh node velocities and (b) retains the resulting predicted (or, if it is known analytically, prespecified) total mass of the system when the dependent variable is recovered on the updated mesh, even when Dirichlet boundary conditions are imposed exactly [3]. The new method can be applied simply to moving boundary problems for which the mass variation is not known *a priori*, e.g. phase change problems. Its application to one- and two-dimensional Stefan problems will be discussed, placing particular emphasis on the approximation of the moving interface (an external boundary for one-phase problems, but internal for two phases). This requires the imposition of both a Dirichlet condition on the dependent variable and the Stefan condition, which models the change of phase by relating the interface velocity to the local solution gradients.

- [1] M.J.Baines, M.E.Hubbard and P.K.Jimack, *A moving mesh finite element algorithm for the adaptive solution of time-dependent partial differential equations with moving boundaries*, Appl. Numer. Math., **54**:450–469, 2005.
- [2] M.J.Baines, M.E.Hubbard, P.K.Jimack and A.C.Jones, *Scale-invariant moving finite elements for nonlinear partial differential equations in two dimensions*, Appl. Numer. Math., **56**:230–252, 2006.
- [3] M.J.Baines, M.E.Hubbard and P.K.Jimack, *Consistent Dirichlet conditions for moving boundary problems*, submitted to Appl. Numer. Math.

Aitken-Schwarz Acceleration with auxiliary background grids

Frank Hulsemann (*EDF R&D*)

Aitken-Schwarz methods are a family of extrapolation based acceleration techniques for Schwarz domain decomposition algorithms. These methods seek to represent or to approximate the so called trace transfer operator, which describes the error propagation from one iteration of the Schwarz DD algorithm to the next. Garbey and Tromeur-Dervout [2,3] have shown that in the best possible case, that is, for separable, linear differential operators and with all eigenvectors of the trace transfer operator and their associated error propagation coefficients at its disposal, the Aitken-Schwarz method converges to the algebraic solution in one extrapolation step.

However, in order to reduce the computational costs of the setup phase, it may not always be desirable to determine all eigenvectors of the trace transfer operator. When the extrapolation is based on an approximation of the trace transfer operator, the Aitken-Schwarz approach loses its direct solver property and turns into an iterative method. In [1], Garbey proposes different ways to approximate the trace transfer operator and gives results to illustrate that the Aitken-Schwarz extrapolation achieves better convergence rates than the non-accelerated Schwarz DD method.

In this contribution, we propose auxiliary background grids as a means to construct approximate trace transfer operators. We apply our approach to grids with refined stripes as a stepping stone towards patch-adaptivity. The method presented here differs from the Aitken-Schwarz "mainstream" in that it uses the extrapolation in a correction scheme and not as a way to represent the algebraic solution. This change of approach, which might seem minor, in fact overcomes convergence problems of the original formulation.

1. Garbey, M., "Acceleration of the Schwarz method for elliptic problems", SIAM J. of Scientific Computing, 26 (6), 1871–1893, 2005.
2. Garbey, M., Tromeur-Dervout, D., "On some Aitken like acceleration of the Schwarz Method", Int. J. for Numerical Methods in Fluids, 40 (12), 1493–1513, 2002.
3. Garbey, M., Tromeur-Dervout, D., "Two Level Domain Decomposition for Multiclusters", in "12th Int. Conf. on Domain Decomposition Methods DD12", Chan, T., Kako, T., Kawarada, H., Pironneau, O. (editors), 325–340, 2001.

IMEX linear multistep methods for stiff hyperbolic relaxation systems

Willem Hundsdorfer & **Steve Ruuth** (*CWI*)

For solving hyperbolic systems with stiff sources or relaxation terms, time stepping methods should combine favorable monotonicity properties for shocks and steep solution gradients with good stability properties for stiff terms. In this paper we consider implicit-explicit (IMEX) multistep methods. Suitable methods will be constructed, based on explicit methods with general monotonicity and boundedness properties for hyperbolic equations. Numerical comparisons are made with several implicit-explicit Runge-Kutta methods.

Stability of ADI schemes for convection-diffusion equations with mixed derivative terms

Karel in 't Hout & **Bruno Welfert** (*University of Antwerp*)

In this talk we are interested in the numerical solution of multi-dimensional convection-diffusion equations where mixed spatial derivative terms are present. Convection-diffusion equations of this kind arise naturally in a variety of areas. For example, in financial mathematics they model the prices of options on a number of correlated assets. The potential use of ADI schemes for the numerical solution of such equations has not yet been explored to great extent in the literature; some promising first results were obtained by McKee & Mitchell (1970), Craig & Sneyd (1988, 1990) and McKee, Wall & Wilson (1996).

In this talk we shall consider three general ADI schemes for the time-integration of semi-discrete multi-dimensional convection-diffusion problems having mixed spatial derivative terms. We present new results on the favourable property of unconditional stability. Numerical experiments are given to illustrate the presence of unconditional stability, as well as showing the actual convergence behaviour of the ADI schemes.

Efficient Meshless Technique for the Solution of KdV Equation.

Siraj Islam & **A. J. Khattak** (*University of Engineering and Technology, Peshawar*)

In this work, we will present a new method based on the radial basis functions to find the solution of Korteweg-de Vries equation. The new form, called controlled RBF, is based on the combination of two radial basis functions controlled by a parameter. In the first controlled RBF, MQ and IQ and in the second IMQ and IQ are used. The new form of

RBFs is best choice to control the ill-conditioning of the RBF system. Numerical results provided shows that we are getting better results by controlled RBF than MQ, IQ and IMQ with smaller condition number.

Adaptive Unstructured High Order Nodal Finite Elements applied to the Bidomain Equations

Nicolas Jeannequin & Jonathan Whiteley, David Gavaghan (*Computing Laboratory, Oxford University*)

We present a novel implementation of a pseudo-spectral scheme on unstructured simplices to solve the bidomain equations. The bidomain model describes the macroscale electrical activity of cardiac tissue and is coupled to a cellular model, such as the Luo-Rudy '91 model (C.H. Luo and Y. Rudy. A model of the ventricular cardiac action potential-depolarisation, repolarisation and their interaction. *Circulation Research*, 68:1501-1526, 1991). The interaction of many different spatial and temporal scales makes this model difficult to solve accurately. We describe an explicit method for the construction of nodes that are suitable for polynomial interpolation on simplices. These nodes are used in our implementation of the pseudo-spectral scheme. They show a performance on par with Fekete (M. Fekete. *Über die verteilung der wurzeln bei gewissen algebraischen gleichungen mit ganzzahligen koeffizienten.* *Math. Zeit.*, 17:228-249, 1923) and electrostatic (J. S. Hesthaven. From electrostatics to almost optimal nodal sets for polynomial interpolation in a simplex. *Siam. J. Num. Anal.*, 35(2):665-676, 1998) nodes up to 12th order, but their very simple construction makes them much more desirable.

The bidomain model is solved using a novel adaptive method in both time and space. All known approaches to time and space adaptivity applied to this problem have concentrated on the use of low order methods. Our spatial discretisation is a high order h-adaptive continuous Galerkin method which is coupled to an adaptive linearly implicit Rosenbrock time integration scheme. This scheme allows the time steps used to be chosen by accuracy considerations rather than stability considerations. The spatial mesh size is determined by the gradient of the transmembrane and extracellular potentials. We also show how to extend this work to a high order h-adaptive discontinuous Galerkin method which is coupled to an adaptive linearly implicit Rosenbrock time integration scheme. Both these approaches are compared in terms of computational time and accuracy.

Efficient algorithms are developed and numerical results show optimal rates of convergence. Computation time of high accuracy numerical computations of the activation speed and propagation speed, which are useful to experimentalists, are greatly reduced when compared to other numerical discretisations. Computational issues associated with this technique such as execution time and memory required are discussed.

Convergence of a RT/DG method for Miscible Displacement Problems

Max Jensen & Soren Bartels, Rudiger Muller (*Durham University*)

We analyse the numerical discretization of a mathematical model describing the single phase, incompressible, miscible displacement of one fluid by another in a porous medium. It is shown under minimal assumptions on the data that the numerical approximations, obtained with a combined mixed finite element and discontinuous Galerkin method in space and an implicit Euler method in time, converge unconditionally to a weak solution of the model problem. Novel features of the analysis are the construction of fully discrete approximations without any regularization of the advection term and a rigorous convergence analysis for the numerical scheme without any regularity or uniqueness assumptions on the exact solutions.

An efficient, adaptive, multigrid solver for phase field models

Peter Jimack & Jan Rosam, Andrew M Mullis (*University of Leeds*)

In recent years the phase field approach has become a popular mathematical tool for the modeling of phase-change problems. The novelty of the approach is that the mathematically sharp interface between the solid and liquid phases is assumed diffuse, allowing the definition of a continuous (differentiable) order parameter, ϕ say, which represents the phase of the material. The evolution of ϕ is governed by a free energy functional which can be solved using standard numerical techniques for PDEs without explicitly tracking the solid-liquid interface, thus allowing the simulation of arbitrarily complex morphologies.

This talk will describe our development of a fully implicit, fully adaptive (in space and time) numerical tool for the solution of phase field equations. Results will be presented for the solidification of a dilute binary alloy requiring solution of the coupled set of equations governing both the evolution of the phase-field and the transport of heat and

mass. Simulating solidification under such conditions is particularly challenging due to the vastly different length scales over which the two diffusion processes operate.

The major advantage of the fully implicit approach that we have now developed is that stiff, highly nonlinear PDE systems, involving very different rates of thermal and solutal diffusion, may be accurately modeled in a computationally efficient manner. The key advance that has permitted this success is the inclusion of a robust multigrid scheme that is able to solve the highly nonlinear discrete equations at each implicit time step in a fast and reliable manner on sequences of locally refined grids.

A fast algorithm for matrix balancing

Phil Knight & Daniel Ruiz (*Strathclyde University*)

As long as a square nonnegative matrix A contains sufficient nonzero elements, then the matrix can be balanced, that is we can find a diagonal scaling of A that is doubly stochastic. A number of algorithms have been proposed to achieve the balancing, the most well known of these being the Sinkhorn-Knopp algorithm. In this talk we derive new algorithms based on inner-outer iteration schemes. We show that the Sinkhorn-Knopp algorithm belongs to this family, but other members can converge much more quickly. In particular, we show that while stationary iterative methods offer little or no improvement in many cases, a scheme using a reconditioned conjugate gradient method as the inner iteration can give quadratic convergence at low cost.

An iterative multi-point flux method with guaranteed positivity

Pantelis Kotzonis (*Oxford University*)

Finite volume numerical methods for the simulation of subsurface flow problems are discussed. In general, full tensor anisotropy effects caused by either non orthogonality of the simulation grid or by the anisotropy of the permeability tensor are observed. When applied to these problems, classical two-point flux schemes such as the ones used in various commercial simulators are generally inconsistent and lead to solutions that are grid dependent - we observe "grid-steering" effects. In recent years multi-point flux approximations (MPFA) have been devised to handle grid distortion and permeability anisotropy in a consistent way. The price to pay for this is an increased flux stencil and a loss of symmetry of the linear operator that arises, while the corresponding continuous operator is itself elliptic and self-adjoint (parabolic in the time dependent

case). In many practical situations multi-point flux schemes actually fail to satisfy the maximum principle, especially when used on strongly distorted grids and highly anisotropic media. As a result, the pressure solution can show errors in the form of spurious oscillations. Many attempts have been carried out to come up with methods that minimize or avoid this phenomenon. A modified iterative multi-point flux method is presented wherein the M-matrix property for the system matrix is guaranteed by an appropriate splitting of the original MPFA matrix. Numerical test examples are presented along with a comparison with the classical MPFA method.

The multi-section method: Why rectangles are sometimes better than squares.

Marko Lindner & Eric Heinemeyer, Roland Potthast (*University of Reading*)

Let A be a bounded and linear operator on a function space E over a (discrete or continuous) unbounded domain. For simplicity, let us restrict ourselves to the one-dimensional domains $\mathbf{Z}$ and $\mathbf{R}$ here, in which case the function spaces we are talking about are of the form $E = \ell^p(\mathbf{Z})$ or $E = L^p(\mathbf{R})$, respectively. In the discrete case, we can think of A as a two-sided infinite matrix $(a_{ij})_{i,j \in \mathbf{Z}}$. In the $L^p(\mathbf{R})$ case we will take integral operators

$$(Au)(x) = \int_{\mathbf{R}} k(x, y) u(y) dy, \quad y \in \mathbf{R}$$

as our model case, where $k(\cdot, \cdot)$ is a suitable function on $\mathbf{R} \times \mathbf{R}$.

We introduce a novel method, the so-called *multi-section method*, for the approximate solution of an equation $Au = f$ in E . The idea is to truncate both the solution u and the right-hand side f to a finite domain, as is usually done with the so-called *finite section method*, but in a slightly different way: We truncate them to two different finite domains and solve the resulting equation only approximately. Roughly speaking, instead of taking a quadratic finite submatrix of $(a_{ij})_{i,j \in \mathbf{Z}}$ or the restriction of $k(\cdot, \cdot)$ to a finite square, we work with rectangular subsections, respectively. This approach was designed to overcome difficulties that one sometimes faces when applying the finite section method.

A finite difference method on layer-adapted meshes for an elliptic system in two dimensions

Torsten Linss & R. Bruce Kellogg, Martin Stynes (*TU Dresden*)

A system of coupled singularly perturbed linear reaction-diffusion equations is considered on the

unit square. An error analysis for the numerical solution of this problem is given for Bakhvalov and Shishkin meshes. This analysis is much simpler than previous analyses of similar problems, even in the case of a single reaction-diffusion equation, as it does not necessitate the construction of an elaborate decomposition of the solution.

This research has been supported by the Boole Centre for Research in Informatics at National University of Ireland, Cork and the Zentrum für Informationsdienste und Hochleistungsrechnen, TU Dresden.

An Unconditionally Stable Second-Order Accurate ALE-FEM Scheme for 2D Convection-Diffusion Problems

John Mackenzie & W.R Mekwi (*Strathclyde University*)

The aim of this talk is to investigate the stability and convergence of time integration schemes for the solution of a finite element semi-discretisation of a scalar convection-diffusion equation defined on a moving domain. An Arbitrary Lagrangian Eulerian (ALE) formulation is used to reformulate the governing equation with respect to a moving reference frame.

By identifying the diffusive and anti-diffusive effects caused by the mesh movement, we devise an adaptive θ -method that is shown to be unconditionally stable and asymptotically second-order accurate. Numerical experiments are presented to back up the findings of the analysis.

A second-order accurate scheme for a fractional wave equation

William McLean & Kassem Mustapha (*University of New South Wales*)

I will discuss a generalized Crank-Nicolson scheme for the time discretization of a fractional wave equation. The scheme uses a non-uniform grid in time to compensate for the singular behaviour of the exact solution at $t = 0$.

Adaptive Multi-Scale Optimisation for Masonry

Angela Mihai & Mark Ainsworth (*University of Cambridge*)

We present an adaptive multi-scale optimisation approach that can be used in predicting the mechanical behaviour of a masonry structure modelled as an elastodynamic frictional multi-body contact problem. This problem is formulated as a non-linear hyperbolic variational inequality and discretised by piecewise polynomial finite elements

in conjunction with an energy consistent time-stepping scheme. At every time-step, the resulting discrete problem is reformulated as a very large-scale non-linear complementarity problem. Currently, methods for efficiently solving dynamic optimisation problems with variational inequality constraints, such as those arising in contact/impact models, are essentially limited. This is due on one hand to the complexity of the governing system of equations and on the other hand to the wide range of space and time scales characteristic to these problems. In our approach, an iterative splitting into normal and frictional contact together with a semismooth Newton procedure is employed to calculate deformations and openings in the model structure. The resulting solution algorithm is then coupled with a dynamic multi-scale technique, based on information from the macroscopic (structural) scale and the mesoscopic (constituents) scale, to account realistically and efficiently for the possible failure of large-scale masonry structures. The support for this work by EPSRC and RSE is gratefully acknowledged.

High Frequency Scattering By Convex Curvilinear Polygons

Moss Mokgolele & S. Langdon, S.N. Chandler-Wilde (*University of Reading*)

Acoustic and electromagnetic wave scattering problems can be formulated as the Helmholtz equation with appropriate boundary conditions. The computational cost of standard schemes for these problems grows in direct proportion to the frequency of the incident wave. Recently Chandler-Wilde and Langdon have proposed a novel Galerkin boundary element method to solve the problem of acoustic scattering by a sound soft convex polygon, with computational cost that depends only logarithmically on the frequency. They achieved this by incorporating into the approximation space the products of plane wave basis functions with piecewise polynomials supported on a graded mesh, with smaller elements adjacent to the corner of the polygon. In this talk we extend their scheme to problems of scattering by curvilinear polygons.

Computation of blowing-up solutions for second order differential equations using rescaling techniques

Nabil Nassif (*American University of Beirut*)

In this paper, we consider the computation of solutions to second order Ordinary Differential Equations of the form:

$$y'' - b|y'|^{q-1}y' + |y|^{p-1}y = 0 \quad t > 0, \\ y(0) = y_{1,0}, \quad y'(0) = y_{2,0}$$

This model describes the motion of a membrane element linked to a spring. The non-linear term in y is related to the rigidity of the spring and that in y' models a “speed-up” of the phenomenon when $b > 0$ and a “slow-down” when $b < 0$. In this last case, the initial-value problem is dissipative and the existence of the solution is global on $[0, \infty)$ ([1], [2]). Computationally, such case is not difficult to handle. However, when $b > 0$, the existence domain of the solution is finite, with the existence of a finite “blow-up time” $T_b > 0$, at which $y(t)$ and $y'(t)$ “explode”, i.e.

$$\lim_{t \rightarrow T_b} |y(t)| = \lim_{t \rightarrow T_b} |y'(t)| = \infty.$$

Such situation can exhibit two types of explosive behavior: Oscillatory, and Non-Oscillatory. In this work, we present a robust algorithm to efficiently compute the solutions to these singular problems. It is based on the idea of “sliced-time” computations introduced in [6], whereby the original system is first written as a system of first-order differential equations, followed by subdividing the interval of existence $[0, T_b]$ into an infinite number of subintervals (slices), with each slice to be determined by the introduction of an “end of slice condition”. For that purpose, we introduce on each slice n^{th} slice, $[T_{n-1}, T_n]$ ($n \geq 1$), a simultaneous change of variables:

$$(t, y_1(t), y_2(t)) \rightarrow (s, z_1(s), z_2(s)).$$

Through such variables change and the use of a “threshold” value S , the equations are modified into a slices-defined set of differential equations.

Numerical results are presented to show evidence of the efficiency of this approach.

- [1] Haraux A. *Systèmes dynamiques dissipatifs et applications*. RMA, vol 17, (1991) Masson, Paris, Milan, Barcelone, Bonn.
- [2] Lasalle J. *Some extensions of Liapunov's second method*, *IRE Trans. Circuit Theory*, CT-7 (1960) 520-527.
- [3] Souplet P. *Critical Exponents, special large-time behavior and oscillatory blow-up in nonlinear ode's* *Differential and Integral Equations*, 11, (1998), 147-167.
- [4] Souplet P. *Etude des solutions globales de certaines équations différentielles ordinaires du second ordre non-linéaires*. C.R. Acad. Sci. Paris, t., 313, Série I (1991), 365-370.
- [5] Souplet P. *Existence of exceptional growing-up solutions for a class of nonlinear second order ordinary differential equations*. *Asymptotic Analysis*, 11 (1995), 185-207.

- [6] N. Nassif, D. Fayad, M. Cortas, *Sliced-time computations with Re-scaling for Blowing-Up solutions to Initial Value Differential Equations*. V.S. Sunderam et al. (Eds.): ICCS 2005, pp. 58-65, Springer-Verlag 2005.

Convergence analysis of planewave expansion for band gap computations in photonic crystal fibres

Richard Norton & Robert Scheichl (*University of Bath*)

Photonic Crystal Fibres (PCFs) are optical fibres that have a core surrounded by cladding. The cladding has a structure that is periodic in the transverse directions of the fibre on a scale comparable with the wavelength of light. We fix the frequency of light and then solve time-harmonic, source free Maxwell's equations for the z-component of the wave vector to determine the modes of light permissible in the fibre. In its most general form this problem is a 2D vector-valued variational eigenvalue problem with piecewise constant coefficient functions.

Following the solution technique of previous work by others we approximate the solution to this problem using the planewave expansion method (spectral Galerkin method). Our research has included the effective implementation of this method as well as the convergence analysis of the errors.

In 1D the problem splits into two problems: the TE mode and the TM mode problem. We have developed complete convergence analysis for the TE mode problem and we will present this theory together with supporting numerical examples that show the results extend to the TM mode problem as well as the 2D version of the TE mode problem.

We have also considered solving a modified problem where the piecewise constant coefficient function, that describes the structure of the PCF, is approximated with a smooth function. We present the convergence analysis for this problem and we answer the question: Is smoothing worth it?

The planewave method requires the Fourier coefficients of our piecewise constant coefficient function. We have considered approximating these Fourier coefficients and we have developed convergence theory for our method of approximation. We also present our results for this case.

Spectral Method for an axisymmetric Stokes Problem

Fatma Zohra Nouri & Mounira Melki (*Laboratoire de Mathématiques Appliquées*)

A well known method for computing viscous incompressible flows in two dimensions relies upon formulating the Stokes problem in terms of the current and whirlpool functions [4] and using the uncoupling strategy proposed by Glowinski and Pironneau in their classical paper on the biharmonic equation [5]. The main motivation of this work is to present a new fitting to formulate this problem. We make use of the analytical results in [1, 3, 6] to investigate the numerical analysis of the discretisation of the Dirichlet problem for Stokes operators in three-dimensional axisymmetric domains by using spectral methods. These methods are specifically associated with quadrature formulas which complete the discretisation of the bilinear form involved in the variational formulation.

References

- [1] K. Amoura and F.Z Nouri, An Algorithm for the Navier-Stokes problem, *Revue Int. ARIMA*, No Spécial TAMTAM'05, Novembre 2006.
- [2] C. Bernardi and M. Dauge and Y. Maday, *Spectral Methods for axisymmetric Problems*, Numerical algorithms and the tests due to Majdi Azaiz (1999), Edition Elsevier Sciences Medicales.
- [3] O. Boutaghou and F.Z Nouri, On Finite Spectral Method for axisymmetric Elliptic Problem, Presented in the Biennial Conference on Numerical Analysis, (Abstract-Dundee, 2001), *F.E. Int. J. of Applied Maths*, Vol 21, 2005.
- [4] V. Girault and P.A Raviart, *Finite Element Methods for Navier-Stokes Equation, Theory and Algorithms*, Springer Verlag, New-York(1986).
- [5] R.Glowinski and O Pironneau, Numerical Methods for the first biharmonic equation, *SIAM SIREV*, Vol 21 No. 2(1979).
- [6] F.Z.Nouri, A New Fitting for a Spectral Method for the solution fo Stokes problem, Presented in the Biennial Conference on Numerical Analysis, (Abstracts, Dundee 1999).

A generic software implementation of lattice sequences for numerical integration

Dirk Nuyens & Ronald Cools (*K.U. Leuven*)

We present an overview on how to implement the very simple formula for the generation of (rank-1) lattice rule points

$$\mathbf{x}_k = \frac{k\mathbf{z} \bmod n}{n}, \quad 0 \leq k < n, \quad \mathbf{z} \in \mathbb{Z}_n^s.$$

These point sets are used for the approximation of s -dimensional integrals by the equal-weight cubature rule

$$\frac{1}{n} \sum_{k=0}^{n-1} f(\mathbf{x}_k) \approx \int_{[0,1]^s} f(\mathbf{x}) \, d\mathbf{x}.$$

Especially in high dimensions, say $s > 100$, lattice rules are an important numerical technique for the approximation of multi-variate integrals, e.g., in mathematical finance. Previous work by the authors involve fast algorithms to construct good generating vectors $\mathbf{z}$ for various kinds of lattice rules.

In its most general form we consider lattice rules with point sets generated as

$$\mathbf{x}_k = \tau(\varphi(k)\mathbf{z}).$$

Hereby is $\varphi(k)\mathbf{z}$ an integer multiple of $\mathbf{z}$ (under the operation of a finite cyclic additive group), τ a mapping from the lattice to the s -dimensional integration domain $[0, 1]^s$ and φ a well chosen permutation to be able to use the lattice rule as a sequence.

The aim of the implementation is for both efficiency and mathematical abstraction. That is: we want to be able to capture the most simple form of a (fixed) lattice rule as well as more involved cases where the lattice is a polynomial lattice and the operation becomes polynomial multiplication, or the point set is to be used as an open sequence. For each possible implementation we want to be able to apply specific optimizations and this without having to hand code each case.

These goals are pursued in C++ in a generic programming style by the use of templates and concepts. In this way it becomes possible to make an abstract mathematical implementation at a high level (being the underlying algebraic structure) and at the same time provide specific optimized implementations where this makes sense. Hence, this presentation shows a case study on how to mix maths and computer science to obtain a usefull (i.e., efficient, reliable, flexible, ...) software library.

On one linear equation in one quaternionic variable

Gerhard Opfer & Drahoslava Janovská (*University of Hamburg*)

Linear equations in only one real or complex variable are not very interesting from an algebraic point of view. But in non commutative algebras, terms of the form ax , xb , cx occur and cannot be combined. In particular, there are singular and non singular linear mappings which, on a first glance, cannot be distinguished. The special case $l(x) := ax + xb$ can be solved completely (i.e. a characterization of the singular cases is possible and a simple solution formula for the non singular cases of $l(x)=e$ will be given). For the more general case $l(x) := ax + xb + cxd$ sufficient conditions for non singularity will be presented. For the even more general case of $l(x) := \sum_{j=1}^m c_j x d_j$ a solution formula for $l(x) = e$ will be given in terms of a simple matrix equivalent. This matrix form is related to the problem of finding the centralizer of a quaternion and its matrix equivalent.

An applications of hybrid of rationalized Haar functions for nonlinear mixed Hammerstein integral equations via a collocation method

Yadollah Ordokhani (*Alzahra University*)

A numerical method for solving nonlinear mixed Hammerstein integral equations is presented in this paper. The method is based upon hybrid of rationalized Haar functions approximations. The properties of hybrid functions which are the combinations of block-pulse functions and rationalized Haar functions are first presented. The operational matrix of integration with the Newton-Cotes nodes and Newton-Cotes integration method are then utilized to reduce the nonlinear mixed Hammerstein integral equations to the solutions algebraic equations. The method is computationally attractive, and applications are demonstrated through illustrative examples.

Analysis of a Quasicontinuum Method

Christoph Ortner & Endre Süli (*University of Oxford*)

The quasicontinuum (QC) method is a finite element based coarse graining technique for atomistic models of solids. The features of atomistic models (long-range interaction, non-convexity, non-uniqueness) make the analysis of the QC method a formidable challenge. In this talk we present a complete a priori and a posteriori analysis in a one-dimensional model problem. We prove under natural conditions that, (i) to any *stable* equilibrium of

the atomistic solid there exists a QC solution which approximates it and (ii) to any *stable* QC solution there exists an equilibrium of the atomistic solid which is approximated by the QC solution.

An invitation to the evolving CHEBFUN system

Ricardo Pachon & Nick Trefethen (*Oxford University*)

CHEBFUN is an object-oriented MATLAB system that approximates functions with very accurate polynomial interpolation. Using ideas of Chebyshev expansions, FFT, barycentric interpolation, Clenshaw-Curtis quadrature and recursive zero-finding, CHEBFUN overloads many of the typical MATLAB commands and allows the user to work in a numerical-symbolic environment. The result is a powerful system to perform numerical computations, not only with numbers but also with functions.

The CHEBFUN system was originally developed by Zachary Battles (Trefethen's DPhil student) during 2002-2006, but new developments have been happening since then. CHEBFUN supports now the definition of piecewise-smooth functions on arbitrary intervals, Dirac's deltas and many other new features. This talk will be both an introduction to the system and a presentation of its new capabilities with examples on approximation theory, differential geometry, analytic continuation and PDE solving.

For more on the CHEBFUN system, visit

<http://web.comlab.ox.ac.uk/projects/chebfun/>

Coupled method of analysis for high order approximations of linear hyperbolic equations and their interfaces and boundaries

Manouchehr Parsaei (*University of Tehran*)

High order approximations of linear hyperbolic equations require complex boundary conditions, interfaces between them are complicated, reflections at the boundaries can occur at multiple frequency ranges and evanescent waves have a more active role. In this paper a method of analysis for high order approximation of linear hyperbolic equations is presented. The method is based on the fact that semi-discretization of hyperbolic equations represents a coupling between independent solutions. A periodic structure in the approximation is sought and manipulated to determine the characteristics and relations between neighboring nodes. This information is valuable when boundaries, interfaces and other effects are examined. By inspecting groups of nodes at a time the coupled method

of analysis can clearly describe the behavior of high order approximations of hyperbolic equations. In 2D approximations some new effects are observed similar to the diffraction phenomenon in optics, they occur when compact differencing is employed and a non-physical obstacle is placed in the flow direction.

Higher-Order Discrete Calculus Methods.

Blair Perot (*University of Massachusetts*)

Discrete calculus methods are an approach in which the PDE system is discretized (transformed into an algebraic system) exactly. This approach results in discrete calculus operators (div, grad, curl) which are exact and therefore obey all the properties (orthogonality, null spaces, etc) of their continuous counterparts. All approximation/errors in discrete calculus methods are restricted to the algebraic material constitutive equations of the PDE.

In this work, the generalization of discrete calculus methods to higher-order is examined. It is shown that on triangular or 2D Cartesian meshes, the underlying function space is the same as higher-order Raviart-Thomas elements. On tetrahedral or 3D Cartesian meshes the Nedelec or face/edge element function space is recovered. However, the test function space is different from classical edge/face elements, and a version of the discrete calculus approach is explored that is akin to a classical finite volume approach or a higher-order unstructured staggered mesh method. The resulting method has a local conservation statement. In addition, like a control volume method, the approach is applicable to general polyhedral meshes and the method does not need shape functions to be explicitly specified, or element shapes and their transformations (to reference elements) to be known. The resulting higher-order operators are shown to have a discrete de Rham complex.

The accuracy and cost of the method is compared to lower order discrete calculus methods, and classical finite volume methods, for a number of simple and complex 3D heat transfer problems on unstructured meshes. The development of these methods was inspired by some of the early works of Griffiths.

J. B. Perot and V. Subramanian, Discrete Calculus Methods for Diffusion, *J. Comput. Phys.*, 224 (1), 59-81, (2007).

J. B. Perot, Conservation Properties of Unstructured Staggered Mesh Schemes, *J. Comput. Phys.*, 159, 58-89. (2000).

D.F. Griffiths, Finite elements for incompressible flow, *Math. Methods in the Appl. Sci.*, 1, 16-31, (1979).

D. F. Griffiths, An approximately divergence-free

9-node velocity element (with variations) for incompressible flow, *Int. J. Num. Meth. Fluids*, 1, 323-246, (1981).

A second-order overlapping Schwarz method for a 2D singularly perturbed semilinear reaction-diffusion problem

Maria Pickett & Natalia Kopteva (*University of Limerick*)

We examine an overlapping Schwarz method for the following semilinear reaction-diffusion boundary-value problem posed on a smooth two-dimensional domain Ω ,

$$Fu = -\varepsilon^2 \Delta u + b(x, u) = 0, \quad x \in \Omega \subset \mathbb{R}^2, \quad (1a)$$

$$u(x) = g(x), \quad x \in \partial\Omega, \quad (1b)$$

where ε is a small positive parameter, b and g are sufficiently smooth and $\Delta = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$ is the Laplace operator. Solutions of such problems can exhibit both boundary and interior layers, however, we will only consider solutions that exhibit boundary layer behavior.

The problem is solved iteratively on two overlapping subdomains Ω_1 and Ω_2 . The overlapping region is of width $O(\varepsilon \ln N)$. In Ω_1 we apply finite difference methods on layer adapted meshes. In Ω_2 we use lumped mass linear finite elements on a quasi-uniform Delaunay triangulation. Discrete sub- and super-solutions are used to prove existence and accuracy of appropriate discrete solutions in the subdomains Ω_1 and Ω_2 . Letting h be the maximum side length of the mesh elements with the number of mesh nodes not exceeding Ch^{-2} , we show that when $\varepsilon \leq Ch$, one iteration is sufficient to obtain second order parameter uniform convergence.

The role of the shape parameter for different RBF methods when solving a convective PDE on a sphere

Cecile Piret & Bengt Fornberg (*University of Colorado*)

In 1990, Ed Kansa pioneered the use of radial basis functions (RBFs) as a method to numerically solve PDEs. This approach has two main advantages: it is typically spectrally accurate, and it is mesh-free. Its accuracy depends on several factors: the type of radial function being used, the value of the radial function's shape parameter and, for time dependent problems, also the integration time. Our test problem will be a convective type PDE on the surface of the sphere. By means of the RBF-QR method, introduced in 2007 by Fornberg and Piret, we are able to explore the resulting accuracy also for small shape parameters (near-flat basis functions), a particularly interesting parameter regime

which has been computationally unreachable until now. The performances of several of the most commonly used radial functions will be compared, both for short and long time integrations. In this context, high smoothness of the radial functions turn out to be of great importance even if the PDE solution itself does not have corresponding smoothness properties. It will be shown that piecewise smooth radial functions, such as cubics, thin plate splines, and Wendland functions do not perform well in this context of solving convective PDEs. This talk will be a natural continuation to both Bengt Fornberg's and Natasha Flyer's talks.

Variable step implementation of ETD methods for semilinear problems

Ana María Portillo & M. P. Calvo (*University of Valladolid*)

Spatial discretization of many evolutionary partial differential equations leads to stiff semilinear systems of ordinary differential equations. Exponential integrators combine the exact solution of the linear part, which is assumed to be responsible of the stiffness of the problem, with the numerical approximation of the remaining non linear terms.

In this talk, we consider a variable step implementation of the *exponential time differencing* (ETD) methods of multistep type derived in [1] and later considered in [2]. A local error estimate of exponential type, whose computation is for free, is introduced and some implementation issues for diagonalizable matrices are addressed. Numerical results showing the behaviour of the proposed variable step implementation are provided as well.

- [1] G. Beylkin, J.M. Keiser & L. Vozovoi, *A new class of time discretization schemes for the solution of nonlinear PDEs*, J. Comput. Phys. **147** (1998) 362–387.
- [2] S. M. Cox & P. C. Matthews, *Exponential time differencing for stiff systems*, J. Comput. Phys. **176** (2002) 430–455.

On the alternative iterations of NEWUOA

Michael Powell (*University of Cambridge*)

NEWUOA is a Fortran package, developed by the author, for unconstrained optimization without derivatives. Most steps in the space of the variables are given by trust region subproblems that employ quadratic models of the objective function, F say. Each model has to interpolate F at about $2n+1$ points, where n is the number of variables, which leaves $n(n-1)/2$ degrees of freedom. It is

taken up when the model is updated by minimizing the Frobenius norm of the change to the second derivative matrix of the model. Thus the work of each iteration of NEWUOA is only of magnitude n squared, which has allowed many problems with more than 100 variables to be solved successfully. There are also alternative iterations, their purpose being to move old interpolation points into suitable new positions, which are also derived in the NEWUOA software from trust region subproblems. Recently, however, some other techniques for picking the new positions have been studied by the author. They require less work than before and also in many numerical experiments they reduce the total number of iterations. These findings will be presented and discussed.

On Adaptive Timestepping using a Stabilised Trapezoidal Rule

Gaurav Prinja & G.K. Prinja, D.J. Silvester (*University of Manchester*)

We study a model parabolic PDE problem and compare two adaptive time stepping methods. One is the stabilised Trapezoidal Rule introduced by Gresho, Griffiths and Silvester (<http://eprints.ma.man.ac.uk/657/>) and the other is an adaptive version of the well known BDF2 method. We also discuss the issue of efficient preconditioning of the linearised equation systems that arise at each time level. In particular we present results computed using a freely available algebraic multigrid solver implemented in a "black-box" fashion within the IFISS MATLAB toolbox (see <http://www.manchester.ac.uk/ifiss>).

The Nearest Correlation Matrix Problem in Finance

Hou-Duo Qi & Defeng Sun (*University of Southampton*)

The talk begins with two examples from finance that can be formulated as the nearest correlation matrix problem. These two examples are the correlation stress testing in determining the value-at-risk of a portfolio and construction of an aggregated correlation matrix for a global market. The talk then moves on to numerical methods. The Lagrangian dual approach is developed for the nearest correlation matrix with not many constraints, while the augmented Lagrangian dual approach is for a large number of constraints. The success of the Newton method in the dual approaches relies on the theory of strongly semismooth matrix-valued functions and the fact that the nearest correlation matrix problem is both primal and dual nondegenerate. Numerical results on real data from Risk-

Metrics database show that the Newton method is fast and robust.

Adaptive Grid Methods for Q-Tensor Theory of Liquid Crystals

Alison Ramage & Christopher J. Newton (*University of Strathclyde*)

In addition to the defect core structure, the dynamics of defect movement is also a crucial issue for liquid crystal cells. Previous numerical simulations of such effects have mostly involved using standard finite difference or finite element techniques on uniform grids, and have often been based on using director theory rather than the **Q**-tensor approach proposed here. However, the presence in the physical problem of characteristic lengths with large scale differences (the size of the defect is very small compared to that of the cell) suggests that more sophisticated numerical modelling techniques could be used to great effect.

One obvious approach is to use an adaptive grid technique, ensuring that there is no waste of computational effort in areas where there is no need for a fine grid. Adaptive grid methods have been successfully used to solve partial differential equations (PDEs) in many branches of computational mathematics such as computational fluid dynamics, mathematical biology, semiconductor modelling and aerospace engineering. In this talk we will present an introductory study of the use of adaptive grid methods for solving PDE problems in **Q**-tensor theory of liquid crystals.

Robust a posteriori error estimation for the nonconforming Fortin–Soulie finite element approximation

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

We obtain a computable a posteriori error bound on the broken energy norm of the error in the Fortin–Soulie finite element approximation of a linear second order elliptic problem with variable permeability. This bound is shown to be efficient in the sense that it also provides a lower bound for the broken energy norm of the error up to a constant and higher order data oscillation terms. The estimator is completely free of unknown constants and provides a guaranteed numerical bound on the error.

Solution of linear ODEs by a pseudo-spectral method with coefficient singularity

Mohammad Rastegari & M. Saravi, R.England, M.T.Bromilow (*University of Shomal*)

In this paper, we first briefly introduce a pseudo-spectral method to solve a linear ODE and then extend it to solve a system of linear ODEs. We consider, in particular, cases where some of the coefficient functions are not analytic and provide some examples.

Stiff ARK Methods

Nicolette Rattenbury (*Manchester Metropolitan University*)

Although Runge-Kutta methods have been important and useful numerical methods for more than 100 years, it is natural to ask how it is possible to generalise them without destroying their essential properties. Approaches to this have taken the form of pseudo Runge-Kutta methods and two-step Runge-Kutta methods. We believe that Almost Runge-Kutta (ARK) methods also have interesting prospects and potential advantages. Although they pass more than one piece of information from step to step they retain the simple stability properties of traditional Runge-Kutta methods. The information that is passed from step to step is in Nordsieck form, ensuring that changing step-size is cheap and convenient.

Most of the research on this class of methods has focused on explicit methods for non-stiff differential equations. In this talk we will introduce Almost Runge-Kutta methods in general, then focus on implicit methods for stiff problems.

Preconditioning iterative methods for PDE constrained optimization

Tyrone Rees & Andy Wathen (*University of Oxford*)

Saddle-point systems arise from most optimization problems with constraints. In this talk I will describe how such problems arise from optimization with constraints which are themselves finite element discretizations of partial differential equations. Such problems are necessarily of very large dimension and matrix factorizations of any type must be avoided. I will describe our initial attempts to precondition such problems and show numerical results on certain test problems.

Partial Solution of Full Symmetric Indefinite Linear Systems

John Reid & Jennifer Scott (*Rutherford Appleton Laboratory*)

For the solution of a sparse indefinite linear system, direct solvers offer a level of robustness that is not available with an iterative solver. A vital component of such a direct solver is a code that

can efficiently perform the partial factorization of a full symmetric indefinite set of equations and the corresponding partial solutions.

In this talk, we will describe a new code for this task. Following our happy experience with the 'block hybrid' format of Andersen et al (2005) in the definite case, we use this here. The format packs the lower-triangular part of the matrix by blocks, each of which is held contiguously in memory and fits into cache. This allows the efficient use of level-3 BLAS.

For stability, we perform interchanges and use 1x1 and 2x2 pivots. These interchanges need not be confined within a single block of the block form, so great care has to be taken with their management to ensure that most of the operations are performed with level-3 BLAS.

B.S. Andersen, J.A. Gunnels, F.G. Gustavson, J.K. Reid, and J. Wasniewski (2005). A fully portable high performance minimal storage hybrid format Cholesky algorithm. ACM TOMS, 31, 201-207.

Limiting accuracy of inexact saddle point solvers

Miro Rozložník & Pavel Jiranek (*Czech Academy of Sciences*)

In this contribution we study numerical behavior of several iterative Krylov subspace solvers applied to the solution of large-scale saddle point problems. Two main representatives of the segregated approach are analyzed: the Schur complement reduction method based on the elimination of primary variables and the null-space projection method which relies on a basis for the null-space represented by the constraints. The success of algorithms for solving the reduced Schur complement or the null-space projected (Hessian) systems depends on the availability of a cheap approximate solution to the inner systems with the diagonal block and/or to the associated least squares problems with the off-diagonal block representing the constraints.

We focus on the question what is the best accuracy we can get from inexact saddle point schemes when implemented in finite precision arithmetic. The fact that the inner solution tolerance strongly influences the accuracy of computed iterates is known and was studied in several contexts such as the framework of inexact Krylov methods and various rounding error analyses. Our approach is based on a standard backward analysis which allows us to take into account both the inexactness of the inner iteration loops as well as accompanying rounding errors that occur in the computation. It appears that the maximum attainable accuracy level in the outer iteration process is mainly given by the inex-

actness of solving the inner problems and it is not further amplified by the rounding errors.

The situation is quite different, if we look at the behavior of residuals associated with the original saddle point system that describe how accurately are the two block equations satisfied (we treat them separately). It is shown that the attainable accuracy of computed approximate solutions depends very much on the back substitution scheme used for computing the other unknown. Independently of the fact that the inner systems are not solved exactly some back-substitution formulas lead ultimately to residuals on the roundoff unit level. Our results confirm that certain implementations deliver approximate solutions which satisfy either the first or the second block equation to the working accuracy. Our analysis thus gives a theoretical explanation for the behavior which was probably observed or it is already implicitly known. The implementations that we point out as optimal are actually those which are widely used and suggested in applications. Our theoretical results are illustrated on a model test example.

This work was supported by the MSMT CR under the project 1M0554 Advanced Remedial Technologies and by the project 1ET400300415 within the National Program of Research "Information Society" and by the Institutional Research Plan AV0Z10300504 "Computer Science for the Information Society: Models, Algorithms, Applications".

Parameter uniform approximations for time-dependent reaction-diffusion problems

Nico Schlömer & Torsten Linss (*TU Dresden*)

The problem in question is the reaction-diffusion equation

$$u_t - \varepsilon \Delta u + cu = f$$

with a small parameter $0 < \varepsilon \ll 1$. Solutions to this type of problems are known to exhibit layers at the boundary of the considered domain. This in turn causes problems for generic discretisation methods and has induced the theory of layer adapted meshes.

In the present context, the Crank-Nicolson method for discretisation in time is used. We derive error estimates in the maximum norm that are uniform with respect to the perturbation parameter ε and improve upon previous results in the literature. For the method in use it is crucial to closely observe the stability of the time discretisation in the maximum norm. A result achieved by Palencia and others serves as a foundation for a deeper analysis that mainly involves resolvent estimates of the kind $\|(z - A_h)^{-1}\|_\infty \leq C/|z|$ in the complex plane.

Anisotropic mesh adaptation based on a posteriori estimates and optimisation of node positions

Rene Schneider & Peter Jimack (*TU-Chemnitz*)

Efficient numerical approximation of solution features like boundary or interior layers by means of the finite element method requires the use of layer adapted meshes. Anisotropic meshes, like for example Shishkin meshes, allow the most efficient approximation of these highly anisotropic solution features. However, application of this approach relies on *a priori* analysis on the thickness, position and stretching direction of the layers. If it is impossible to obtain this information *a priori*, as it is often the case for problems with interior layers of unknown position for example, automatic mesh adaption based on *a posteriori* error estimates or error indicators is essential in order to obtain efficient numerical approximations.

Historically the majority of work on automatic mesh adaption used locally uniform refinement, splitting each element into smaller elements of similar shape. This procedure is clearly not suitable to produce anisotropically refined meshes. The resulting meshes are over-refined in at least one spatial direction, rendering the approach far less efficient than that of the anisotropic meshes based on *a priori* analysis.

Automatic anisotropic mesh adaption is an area of active research. Here we present a new approach to this problem, based upon using not only an *a posteriori* error estimate to guide the mesh refinement, but its sensitivities with respect to the positions of the nodes in the mesh as well. Once this sensitivity information is available, techniques from mathematical optimisation can be used to minimise the estimated error by moving the positions of the nodes in the mesh appropriately.

The basic idea of minimising an error estimate is of course not new, but the approach taken to realise it is. The discrete adjoint technique is utilised to evaluate the sensitivities of an error estimate, reducing the cost of this evaluation to solving one additional equation system. This approach is crucial to make gradient based optimisation techniques, such as BFGS-type schemes, applicable. For more details, see

- [1] R. Schneider and P.K. Jimack, *Toward anisotropic mesh adaption based upon sensitivity of a posteriori estimates*, School of Computing Research Report Series 2005.03, University of Leeds, 2005.
http://www.comp.leeds.ac.uk/research/pubs/reports/2005/2005_03.pdf

The performance of a new HSL out-of-core solver

Jennifer Scott & John Reid (*Rutherford Appleton Laboratory*)

A key strength of the mathematical software library HSL and one for which it is internationally renowned is its collection of packages for the direct solution of sparse linear systems of equations. Direct methods are popular for their robustness and efficiency. Their main weakness is that the memory they require usually increases rapidly with problem size. One way of attempting to overcome this limitation is to use a solver that is able to hold its data structures on disk, that is, an out-of-core solver. We have designed and developed a new multifrontal solver called HSL_{MA77}. It relies on direct-access files to hold the original matrix, its factorization, and the bulk of its intermediate data. The first release of the code is for positive definite symmetric systems; we are currently developing versions for indefinite symmetric systems and for unsymmetric finite element systems.

In this talk, we give a brief overview of HSL_{MA77} and present numerical results for a range of large-scale problems arising from practical applications. It is shown that the overhead for out-of-core working in our tests is less than 25 per cent of the solution time. Furthermore, when run in-core, HSL_{MA77} generally outperforms other HSL direct solvers for large positive definite systems.

Efficient Implementation of the One-Sided Indefinite Block Jacobi Method

Sanja Singer & Vjeran Hari and Saša Singer (*University of Zagreb*)

Besides accuracy, a modern eigenvalue algorithm should also have comparable efficiency with other algorithms for the same purpose.

We show how to improve the performance of the one-sided indefinite Jacobi method for computing hyperbolic singular values of rectangular matrices. Combined with the Hermitian indefinite factorization, this method is an accurate eigensolver for Hermitian indefinite matrices.

The main idea of our block algorithm is to work with block-columns to take advantage of the cache memory. There are many choices of annihilation strategies, which can be divided into two groups — the *block-oriented* and the *full block* strategies. In both cases, special care has to be taken to assure the overall quadratic convergence.

For large matrices our block algorithms can be 50% faster than their simple (non-blocked) counterparts. We also show that the proposed algorithms inherit the relative accuracy from the simple one-

sided indefinite Jacobi algorithm.

Orthosymmetric Block Reflectors

Sasa Singer & Sanja Singer (*University of Zagreb*)

We develop a general theory of reflectors and block reflectors in a class of non-Euclidean scalar product spaces generated by orthosymmetric scalar product matrices J , i.e.,

$$J^* = \tau J, \quad \tau \in \mathbf{F}, \quad |\tau| = 1,$$

where $\mathbf{F} = \mathbf{R}$ or $\mathbf{F} = \mathbf{C}$. Reflection and mapping properties of these J -reflectors are studied in detail. Block J -reflectors can be used for block annihilation in QR-like factorizations, where Q is J -unitary and R is block upper triangular. As an example, we consider the general case of the hyperbolic QR factorization.

A Numerical Scheme for a Parameterized Singularly Perturbed Differential Equation.

Meghan Stephens & Niall Madden (*National University of Ireland, Galway*)

We consider a singularly perturbed, second order differential equation: *find a function u and positive parameter κ which satisfy*

$$-\varepsilon^2 u''(x) + a(x, \kappa)u(x) = 0, \quad x \in (0, 1), \quad (2)$$

$$u(0) = 0, \quad u(1) = f(\kappa) \geq 0, \quad (3)$$

$$g(u'(1), \kappa) = 0. \quad (4)$$

It is well known that, for a fixed κ and $0 < \varepsilon \ll 1$, the solution to (2)–(3) may exhibit layers in which the solution changes rapidly. The accuracy of a numerical scheme to solve (2)–(4) will depend not only on an estimate of u inside the layer but also on an estimate of $u'(1)$. A uniform mesh produces an accurate approximation outside the layer, but does not resolve the boundary layer. Moreover, any estimate for the $u'(1)$ will be quite inaccurate. Therefore, a uniform mesh cannot be used with an iterative procedure to solve (2)–(4).

We present an iterative scheme, based on a piecewise uniform “Shishkin” mesh that does accurately solve (2)–(4), and give supporting numerical results.

The use of correlated observation errors in data assimilation

Laura Stewart & Sarah Dance, Nancy Nichols (*University of Reading*)

Data assimilation provides techniques for combining observations and prior model forecasts to create

initial conditions for numerical weather prediction (NWP). The relative weighting assigned to each observation in the analysis is determined by its associated error. Remote sensing data usually has correlated errors, but the correlations are typically ignored in NWP. Recent technological advances have challenged the practicality of these assumptions. For example, high spatial resolution data collected from satellites is now needed to initialise high resolution models designed to better forecast convective storms.

Here we describe three approaches to the treatment of observation error correlations. For an idealised data set, the information content under each simplified assumption is compared to that under the correct correlation specification. Treating the errors as uncorrelated results in a significant loss of information. However, retention of an approximated correlation gives clear benefits.

Combination preconditioning and self-adjointness in non-standard inner products with application to saddle point problems

Martin Stoll & Andy Wathen (*Oxford University*)

In 1988 Bramble and Pasciak showed that if the symmetric indefinite saddle point matrix of the form

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

is preconditioned by the block lower triangular matrix

$$\mathcal{P} = \begin{bmatrix} A_0 & 0 \\ B & -I \end{bmatrix}$$

the resulting preconditioned matrix $\hat{\mathcal{A}} = \mathcal{P}^{-1}\hat{\mathcal{A}}$ is self-adjoint in the inner product defined by the matrix

$$\mathcal{H} = \begin{bmatrix} A - A_0 & 0 \\ 0 & I \end{bmatrix};$$

certain conditions on A_0 guarantee that $\mathcal{H}$ is positive definite. Hence, the Conjugate Gradients method can be applied.

In 2006 Benzi and Simoncini derived a completely different method where under certain conditions the preconditioned saddle point system is symmetric and positive definite in a non-standard inner product.

These methods seem like isolated events where a non-standard inner product ensures the applicability of a short term recurrence method for a non-symmetric matrix. We will show how appropriate preconditioners and inner products can be combined based upon some basic mathematical observations for self-adjoint matrices which will enable the use of short-term recurrence methods such as

CG or MINRES . We will further show the application to saddle point systems where in particular the combination of the Bramble-Pasciak setup and the Benzi and Simoncini configuration will be illustrated.

A new radial basis set for the Schrödinger equation in spherical coordinates.

Tor Sørøvik & Tore Birkeland and Gabriel Oksa
(*University of Bergen*)

A popular technique for solving the time dependent Schrödinger equation is using a split operator technique for time stepping and spectral approximation in space. In Cartesian coordinates the Fourier basis is usually a good choice. However, when the physics are best represented in (hyper)spherical coordinates, accurate approximation by a Fourier expansion in the radial direction, usually require an excessive amount of basis functions.

Here we present an alternative spectral approximation scheme based on a variable transformation $[0, \infty) \mapsto [-1, 1)$ combined with a basis of Chebyshev polynomials. For some problems the new basis set gives order of magnitude faster computation for results of comparable accuracy. While for other problems the standard technique do better. This is illustrated and explained through computational experiments.

A Hybrid of the GMRES method and Electromagnetism Meta-Heuristic method for (nearly) singular systems

Seyyed Hassan Taheri & Faezeh Toutounian
(*Ferdowsi University of Mashhad*)

GMRES is a popular iterative method for the solution of large linear systems of equation with a sparse nonsingular matrix. When A is singular or nearly so, i.e., ill conditioned, GMRES may breakdown before an acceptable approximate solution has been determined. This paper presents a hybrid of GMRES method and Electromagnetism Meta-Heuristic method to overcome the breakdown. Both consistent and inconsistent systems are considered. Numerical examples are used to show the good numerical properties.

Introduction to Compressed Sensing

Jared Tanner & David Donoho (*University of Utah*)

Compressed Sensing is a revolutionary sampling technique where the number of measurements of data needed is proportional to the information content in the signal, rather than the overall space the signal might be contained in. Compressed Sensing

was introduced by David Donoho in late 2004, with similar results independently developed by Candes and Tao at the same time. The essential points of this important new theory will be presented.

CONTEST: A Controllable Test Matrix Toolbox for MATLAB

Alan Taylor & Des Higham (*University of Strathclyde*)

Large, sparse networks appear across a variety of scientific disciplines, including bioinformatics, computer science and the social sciences. Investigating such networks typically reduces to tasks in matrix computation, and these problems are challenging due to the size and lack of regular structure in the resulting matrices. In order to test the robustness and efficiency of matrix computation methods, it is desirable to have a large number of synthetic test matrices that capture key properties of real life systems. CONTEST is a random network toolbox for MATLAB that implements various random graph models, that is, algorithms for randomly assigning edges in a network, that aim to produce realistic connectivity patterns. In addition to adjacency matrices, the toolbox also generates the coefficient matrices in the accompanying linear system and eigenvalue problems that arise for typical tasks such as clustering, ordering, ranking and computing mean hitting times.

The history of random graph models dates back to the seminal 1950s work by Erdős and Rényi, and received substantial impetus from a 1998 paper in *Nature* by Watts and Strogatz that introduced the concept of a *small world* network and a 1999 paper in *Science* by Barabási and Albert that focused on the *scale free* property.

In this talk, we will provide some background into random graph models, and show how the CONTEST toolbox can be used to construct realistic, challenging sparse test matrices.

This is joint work with Des Higham.

On Ideal and Worst-case GMRES

Petr Tichy & J. Liesen, V. Faber (*Institute of Computer Science, Academy of Sciences of the Czech Republic*)

The convergence analysis of the GMRES method for solving linear algebraic systems $Ax = b$ is still an open area of research. If A is normal, then GMRES solves a certain approximation problem on the spectrum of A . For nonnormal matrices the situation is much less clear. A possible approach in the nonnormal case is to concentrate on the *ideal* GMRES approximation $\varphi_k(A)$ that represents an

upper bound on the *worst-case* GMRES residual norm $\psi_k(A)$,

$$\begin{aligned}\psi_k(A) &\equiv \max_{\|v\|=1} \min_{p \in \pi_k} \|p(A)v\| \\ &\leq \min_{p \in \pi_k} \|p(A)\| \equiv \varphi_k(A).\end{aligned}\quad (5)$$

Some nonnormal matrices A are known with $\psi_k(A) < \varphi_k(A)$ for certain k . However, it is still unknown whether $\psi_k(A) = \varphi_k(A)$, or at least $\psi_k(A) \approx \varphi_k(A)$ for larger classes of nonnormal matrices.

In this talk we study the relation between ideal and worst-case GMRES. We summarize known results and prove that worst-case GMRES starting vectors satisfy so called “cross equality”. This phenomenon has been first observed by Zavorin in his Ph.D. thesis. We also present our latest results on ideal and worst-case GMRES for a Jordan block.

Hypercomplex vorticity representation of fluid flow

Leonardo Traversoni (*Universidad Autonoma Metropolitana*)

We present a numerical representation of incompressible fluid flow using the quaternionic formulation of vorticity.

We show that doing so our problem, instead of being to solve PDE’s, is an interpolatory problem and we propose some numerical solutions that we claim can be easier to implement than traditional methods.

Robust Coarse Spaces for Domain Decomposition Methods

Jan Van lent & Ivan Graham, Robert Scheichl (*University of Bath*)

Two-level overlapping Schwarz methods for elliptic equations combine one level of local solves on overlapping domains with a global solve of a coarse approximation of the original problem. To obtain robust methods for equations with highly varying coefficients, it is important to carefully choose the coarse space used to construct this approximation. Inspired by methods for the one-dimensional problem formulated using energy minimization, Wan Chan and Smith [1] proposed a coarse space based on a constrained energy minimization problem. This approach is supported by recent theory on the convergence of Schwarz methods that takes into account coefficient variation [2]. The Lagrange multipliers for the constrained minimization problem are found by solving a large linear system. The coarse basis functions are then found by solving local systems.

Xu and Zikatanov [3] showed that, for multigrid methods, the system for the Lagrange multipliers can be solved efficiently using an appropriate preconditioner. They hint at a preconditioner for the domain decomposition case, but only present a Jacobi preconditioner, which is not robust for two-level Schwarz methods applied to equations with highly varying coefficients. We propose a preconditioner for the domain decomposition case, discuss how it can be implemented efficiently and demonstrate that it is robust. The resulting approach provides an algebraic way to construct a robust two-level overlapping Schwarz method given only the system matrix and the matrices representing the local spaces for the one-level method.

- [1] W. L. Wan, T. F. Chan, and B. Smith, *An energy-minimizing interpolation for robust multigrid methods*, SIAM J. Sci. Comput., 21(4), pp. 1632–1649, 2000.
- [2] I. G. Graham, P. Lechner, and R. Scheichl, *Domain Decomposition for Multiscale PDEs*, BICS Preprint 11/06, Bath, 2006.
- [3] J. Xu, and L. Zikatanov, *On an energy minimizing basis for algebraic multigrid methods*, Comput. Vis. Sci., 7(3–4), pp. 121–127, 2004.

P-stable Obrechhoff methods of arbitrary order for second-order differential equations

Guido Vanden Berghe & M. Van Daele (*Ghent University*)

Following the ideas of Ananthakrishnaiah we develop a family of P-stable Obrechhoff methods of arbitrary even order. The coefficients of these methods follow from a recursive algorithm. It is also shown that the stability functions of the thus obtained methods can be expressed as Padé approximants of the exponential function with a complex argument. A numerical example is given to illustrate the performance of the methods.

- [1] U. Ananthakrishnaiah, *P-stable Obrechhoff Methods with Minimal Phase-Lag for Periodic Initial Value Problems*, Math. Comput. 49 (1987), 553–559.
- [2] U. Ananthakrishnaiah, *Adaptive methods for periodic initial value problems of second order differential equations*, J. Comput. Appl. Math. 8 (1982), 101–104.
- [3] M. Van Daele and G. Vanden Berghe, *P-stable Obrechhoff methods of arbitrary order for second-order differential equations*, Numerical Algorithms (2007)(in press)

A local restart procedure for iterative projection methods for nonlinear symmetric eigenproblems

Heinrich Voss & Marta Betcke (*Hamburg University of Technology*)

We consider the nonlinear eigenvalues problem $T(\lambda)x = 0$ where $T(\lambda) \in C^{n \times n}$ is a family of large and sparse matrices depending on a real parameter λ . Similarly to linear problems, iterative projection methods of Arnoldi and of Jacobi–Davidson type have turned out to be efficient. Here approximations to the wanted eigenvalues and eigenvectors are obtained from projections of the eigenproblem to subspaces of small dimension which are expanded in the course of the algorithm.

A crucial point in these methods for general nonlinear eigenvalue problems when approximating more than one eigenvalue is to inhibit the method to converge to the same eigenvalue repeatedly. However, if the underlying large problem is symmetric such that its eigenvalues satisfy a minmax characterization, then this property is inherited by the projected problems, and the eigenvalues can be determined safely one after the other by safeguarded iteration.

This approach hits its limitations if a large number of eigenvalues (in particular in the interior of the spectrum) is needed, since in this case one has to project the problem under consideration onto a sequence of search spaces of growing dimensions requiring an excessive amount of storage and computing time. In this presentation we propose a new local restart technique which projects the eigenproblem only to search spaces of limited dimension. Our presentation is restricted to the Arnoldi method, but the local restart technique applies also to any other iterative projection method. Its efficiency is demonstrated by a large conservative gyroscopic eigenvalue problem which models the behavior of a rotating tire.

A modification of the computer software should follow the new computer hardware

Jerzy Wasniewski & B.S. Andersen, F. Gustawson, J. Gunnel and J.K. Reid (*Danish Technical University*)

The standard of DLAS (Dense Linear Algebra Software) is the Lapack and ScaLapack libraries. They are supported by level 1, 2 and 3 BLAS (Basic Linear Algebra Subprograms) and the BLACS (Basic Linear Algebra Communication Subprograms). These software followed earlier standard software named LINPACK and EISPACK. LINPACK and EISPACK followed the Wilkinson and Reinsch *Handbook for automatic computation*,

and Forsythe, Malcolm and Moler *software books*. There are also many other very good DLAS library packages.

The hardware of HPC (High Performance Computers) are ever changing, and new performance features appear with each new platform. The above software can have its performance improved by modification that support these new features. A challenge for HPC is to incorporate these new features while maintaining validity and robustness of these existing standard software. New versions of Lapack and ScaLapack libraries are being developed.

As an example of this process we demonstrate performance improvements of the DLAS for symmetric matrices.

Preconditioning for self-adjointness

Andy Wathen & Martin Stoll (*Oxford University*)

It is widely appreciated that the iterative solution of linear systems of equations is much more reliable when the coefficient matrix is symmetric. The Conjugate Gradient and MINRES algorithms are methods of choice which are underpinned by descriptive convergence theory that gives clear guidance on desirable preconditioners to enable rapid convergence. For nonsymmetric matrices there are no generally descriptive estimates and many available methods: GMRES, BICGSTAB, QMR,... which are used in various applications.

In this talk I will consider examples - in particular an important situation derived by Jim Bramble and Joe Pasciak - where preconditioning can be used to give self-adjoint matrices in non-standard inner products. Thus symmetric iterative methods can be employed in such an inner product with the consequent benefits. Extensions of this idea will also be shown.

Fitting linear manifolds using orthogonal distances

Alistair Watson (*Dundee University*)

Let data points $x_i \in R^n, i = 1, \dots, m$, be given. Of interest here is the problem of fitting to these a d -dimensional linear manifold, by minimizing a norm of the vector of orthogonal distances from the points to the manifold. Important special cases are the fitting of lines, planes and enclosing cylinders in R^3 , and such problems arise in computational metrology, geometry, computer vision and robotics. A simple iterative algorithm is presented.

The Kink Phenomenon in Fejér and Clenshaw–Curtis Quadrature

Andre Weideman & L.N. Trefethen (*University of Stellenbosch*)

The Fejér and Clenshaw–Curtis rules for numerical integration exhibit a curious phenomenon when applied to certain analytic functions. When N (the number of points in the integration rule) increases, the error does not decay to zero evenly but does so in two distinct stages. For N less than a critical value, the error behaves like $O(\varrho^{-2N})$, where ϱ is a constant greater than 1. For these values of N the accuracy of both the Fejér and Clenshaw–Curtis rules is almost indistinguishable from that of the more celebrated Gauss–Legendre quadrature rule. For larger N , however, the error decreases at the rate $O(\varrho^{-N})$, i.e., only half as fast as before. Convergence curves typically display a kink where the convergence rate cuts in half. In this talk we present explicit as well as asymptotic error formulas that provide a description of this phenomenon.

A Finite Element Method for Immiscible Fluid Flow

Richard Welford & David Kay and Vanessa Styles (*University of Sussex*)

A fully practical finite element method for a phase field model of immiscible fluid flow is presented, along with a new nonlinear multigrid scheme for solving the resulting discrete problem. The problem we solve consists of a coupled system of Cahn–Hilliard and Navier–Stokes equations. Some analysis of the system and numerical results are also presented.

Numerical solution of nonlinear ODEs and PDEs by using multiwavelet

Sohrab Ali Yousefi & S.E. Banifatemi (*Shahid Beheshti University*)

A numerical method for solving nonlinear ordinary and partial differential equations is presented. The method is based upon Legendre Multiwavelets approximations. The properties of Legendre Multiwavelets are first presented. These properties together with the Gaussian integration method are then utilized to reduce the nonlinear ordinary and partial differential equations to the solution of algebraic equations. Illustrative examples are included to demonstrate the validity and applicability of the technique.