

**THE INSTITUTE OF MATHEMATICS AND ITS
APPLICATIONS**

IMANA NEWSLETTER

**Newsletter of the Numerical Analysis Group of the
Institute of Mathematics and its Applications**

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1 Comments and miscellaneous news

We start with some great news. On Monday 11 August 2008, **Professor Roger Fletcher FRS FRSE** of the University of Dundee was presented with a **Royal Gold Medal** (one of three awarded this year) by the Duke of Edinburgh at The Palace of Holyroodhouse. The Medallists are recommended by the Royal Society of Edinburghs Council, in recognition of intellectual endeavour which has had a profound influence on peoples lives, world-wide. The citation for Roger's medal reads: "The reputation of applied and computational mathematics in Scotland has benefited enormously from the presence of Roger Fletcher, and it is for this outstanding contribution that he is being awarded a Royal Medal." There are more details at <http://www.maths.dundee.ac.uk/info/rogerprize.shtml>. Very many congratulations to Roger for this highly deserved award.

A notable anniversary this year is the **25th Anniversary of The Institute for Computational Fluid Dynamics (ICFD)**. The ICFD was founded in 1983 by Bill Morton and Mike Baines. To celebrate its 25th anniversary a two day meeting was held at the University of Oxford on 15th and 16th September 2008. The meeting consisted of invited talks together with a celebratory 3-course dinner in New College on the evening of 15th September. The full programme and some of the talks can be viewed on line at <http://www.icfd.rdg.ac.uk/ICFD25/index.htm>; more information on the ICFD is available at <http://www.icfd.rdg.ac.uk/>

News flash: Iain Duff writes "During the PRACE Petascale Summer School held in Stockholm on August 26th-29th, Xavier Pinel and Xavier Vasseur from the Parallel Algorithms Team at CERFACS successfully ported a three-dimensional Helmholtz solver to the IBM Blue Gene P at Juelich, Germany and the CRAY XT4 at Espoo, Finland. They showed almost perfect scalability on up to 65,536 cores both in the weak sense (when the computation per processor is kept constant) and in the strong sense (when the same problem is run on an increasing number of processors) on academic model problems. They were able to solve a linear system of **68 billion unknowns in less than 3 hours** setting a new benchmark for the solution of large sparse indefinite systems. The PhD thesis of Xavier Pinel is funded by TOTAL and cosupervised by Serge Gratton (CNES/CERFACS) and Xavier Vasseur. This work is in collaboration with Henri Calandra at TOTAL."

Gabriel Lord (Heriot-Watt) would like to draw the attention of readers interested in stochastic differential equations and numerics to the **SDE-Net** hosted by Heriot-Watt University. Full details are available at <https://list-serve.hw.ac.uk/mailman/listinfo/sde-net> Subscribers receive a plain text digest of announcements of meetings, new books or journals, jobs, software, etc related to stochastic differential equations and applications.

In this issue of the Newsletter, we continue our series of articles that aim to introduce the members, interests and activities of NA groups in the UK, with a look at the group I lead at the Rutherford Appleton Laboratory (with thanks to Sue Dollar). In addition, we have reports by David Silvester (Manchester) on the very successful LMS Durham Symposium that was held in July and by Jan van Lent (Bath) on the annual Bath/RAL Numerical Analysis Day. In the software section, Nick Trefethen (Oxford) introduces us to his chebfun project.

Finally, I would like to draw your attention to a very special two-day meeting to be held next summer entitled **Sparse Matrices for Scientific Computation: In Honour of John Reid's 70th Birthday**. Many of you will know John, an eminent UK numerical analyst with a career spanning five decades. The aim of this meeting is to bring together leading numerical analysts from the UK and abroad in honour of his 70th birthday. The meeting will be held at the Cosener's House in Abingdon, close to Oxford (www.scitech.ac.uk/About/Find/Coseners/Introduction.aspx). Further details will follow in the next Newsletter and will be made available at <http://www.numerical.rl.ac.uk/people/hsd/jkr/>

The copy date for the next Newsletter will be **Wednesday 17th December**. As always, regular or one-off contributions from individuals and from NA groups are very welcome. Comments, feedback, and ideas for articles are also welcome. In particular, if you have any suggestions for an article that you feel would be of interest to readers, please send me an email or give me a call.

Jennifer Scott (j.a.scott@stfc.ac.uk)
Group Leader, Numerical Analysis Group
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2 Meet the Numerical Analysis Group ... RAL

The Numerical Analysis Group originally started its life at the Harwell Laboratory and not the Rutherford Appleton Laboratory. In the early 1970s, the Computer Science and Systems Division was formed from part of the Theoretical Physics Division at Harwell. At the same time, following a partitioning of Alan Curtis's Applied Mathematics Group, the Numerical Analysis Group was born with Mike Powell being the Group Leader. In 1975, Mike moved to Cambridge and John Reid became the Group Leader. Eleven years later, Iain Duff took over the position. In 1990, the Group underwent a large change when it moved from Harwell to the Rutherford Appleton Laboratory (situated next door to the Harwell Campus and now part of the Computational Science and Engineering Department of the Science and Technology Facilities Council (STFC)). Iain remained the Group Leader until 2007, when he handed over to Jennifer Scott. Since 1999, the Group has been funded by a series of EPSRC grants.

The Group is nationally and internationally recognised for both its research and software in numerical linear algebra and numerical optimization. The Group's important scientific achievements include sparse direct methods (for example, frontal and multifrontal methods, novel ordering schemes for sparse matrices, partitioning techniques), stopping criteria for iterative methods, and the design and analysis of methods for unconstrained and constrained optimization, with special interests in conjugate-gradient and other methods for sparse non-convex quadratic programming. In terms of software, the Group has developed the HSL, LANCELOT and GALAHAD libraries; sparse matrix test sets; CUTEr, the de facto optimization test set; and also worked on BLAS and sparse BLAS.

The internationally renowned HSL library was formerly called the Harwell Subroutine Library and, as the name suggests, was originally developed at the Harwell Laboratory. The Library was started in 1963 and it had its first external customer in 1964. Amongst its best known packages are those for solving sparse linear systems, optimization and sparse eigenvalues. HSL software is available without charge to individual academic users for their personal (non-commercial) research and for teaching.

The award-winning nonlinear optimization package LANCELOT was developed in the early 1990s by Nick Gould and his collaborators Andy Conn (IBM) and Philippe Toint (Namur). LANCELOT was succeeded by an on-going general library of packages for optimization, GALAHAD, in 2003, with Dominique Orban (Montreal) joining the collaboration. Testing optimization software necessitated the development of CUTE (later CUTEr) an evolving large collection of realistic optimization examples along with evaluation tools.

The Group has close links with a number of universities. For example, members of the Group provide MSc courses at the Universities of Oxford and Reading, are involved in the supervision of CASE students at the Universities of Bath and Oxford, and are visiting professors at a number of universities. Since its Harwell days, the Group has run a joint seminar series with the Computing Laboratory in Oxford and for the last seven years has jointly organised an annual Numerical Analysis Day with the University of Bath.

The current members of the Group are:

Mario Arioli was a visitor at Harwell in 1986 and 1987. He has been a Group member since 2000.

His main areas of interest are error analysis, stopping criteria for iterative methods, novel iterative methods and domain decomposition methods.

Sue Dollar joined the Group in 2006 following a temporary lectureship at the University of Reading.

Prior to that she was a D.Phil student at Oxford which is when she started to collaborate with the Group. Her main areas of interest are the solution of saddle-point problems, preconditioning methods, PDE-constrained optimization and ordering schemes for sparse matrices.

Iain Duff has been a Group member since 1975. He was Group leader for over twenty years (from 1986) and is a Senior Fellow of the STFC. He is also the leader of the Parallel Algorithms Project at CERFACS, Toulouse, a Fellow of the Royal Society of Edinburgh, and a visiting professor at the University of Strathclyde. Iain is chair of the SIAM Board and a member of the Applied Mathematics Panel for RAE 2008. His main areas of interest are in sparse matrices, direct and hybrid methods, parallel computation and mathematical software.

Nick Gould joined the Group in 1985 and is a Fellow of the STFC. He is also a visiting professor at both the Universities of Edinburgh and Oxford. Nick supervises **Daniel Robinson**, a

postdoctoral researcher on the EPSRC-funded grant “Algorithms for large-scale nonlinearly constrained optimization”. His main areas of interest are optimization, complexity, saddle-point systems and mathematical software.

Jonathan Hogg joined the Group in January 2008 for twelve months as a research assistant on the EPSRC grant “Enhancing HSL for HPC architectures”. In January 2009, Jonathan will return to the University of Edinburgh to complete his PhD in the Operational Research and Optimization Group.

John Reid joined the Group in 1969 and was the Group Leader from 1975 to 1986. He ceased to be a full member of the Group on his retirement in 1998, but since then has continued to play a very active role as a part-time consultant. Currently, his main research interests are numerical linear algebra and, in particular, direct methods for sparse matrices. He is Convener of the ISO/IEC Fortran committee (Fortran is used for all the Group’s codes) and a visiting professor at Cranfield University.

Jennifer Scott joined the Group in 1987. In 2007 she became the Group Leader. Jennifer is a Fellow of the IMA, a member of the Women in Mathematics Committee of the London Mathematical Society, the UK representative of European Women in Mathematics, and a member of the National Coordinating Committee for Women in Science, Engineering and Construction. Her main areas of interest are direct and iterative methods for sparse linear systems, sparse eigenvalue systems, parallel computing, large-scale scientific computation and mathematical software.

More information can be found at www.cse.scitech.ac.uk/nag/index.shtml

Sue Dollar (sue.dollar@stfc.ac.uk).

3 Academic prizes: calls for submissions

14th Leslie Fox Prize

The Fourteenth Leslie Fox Prize meeting will take place on 29 June 2009, at the Mathematics Institute, University of Warwick.

Entries for the Fourteenth Leslie Fox Prize competition can now be submitted. Any person who is less than 31 years old on 1 January, 2009 and has not already won a first prize is eligible. Each entry should consist of a paper, describing some of the candidate’s research, that is suitable for a 40 minute lecture at a numerical analysis meeting.

The entries will be considered by an Adjudicating Committee of Andrew Stuart (Warwick, Chairman), Mark Ainsworth (Strathclyde) and Nick Higham (Manchester). Entries should be received, by the Chairman, by **31 January, 2009**, either electronically as a pdf file, or as three hard copies by regular mail. The receipt of all entries will be acknowledged.

Full details of the prize, and the submission procedure, may be found at: <http://www.warwick.ac.uk/masdr/fox/>

Germund Dahlquist Prize

The Germund Dahlquist Prize is awarded to a young scientist (normally under 45) for original contributions to fields associated with Germund Dahlquist, especially the numerical solution of differential equations and numerical methods for scientific computing.

The Dahlquist Prize will be awarded at SciCADE09, to be held May 25-29, 2009, in Beijing, China. The award consists of a certificate and a cash award of 1000US dollars. The recipient is expected to give a lecture at the meeting. SIAM will reimburse the recipient’s travel expenses to attend the meeting and deliver the lecture.

Nominations should be addressed to Professor Desmond J. Higham, Chair, Germund Dahlquist Prize Committee and sent by **15 October 2008**, to J. M. Littleton at littleton@siam.org. Enquiries should be addressed to littleton@siam.org. See also www.siam.org/prizes/nominations.php.

James H. Wilkinson Prize

The James H. Wilkinson Prize in Numerical Analysis and Scientific Computing is awarded every four years for research in, or other contributions to, numerical analysis and scientific computing during the six years preceding the award. The purpose of the prize is to stimulate junior contributors and to help them in their careers.

SIAM will award the Wilkinson Prize at the SIAM Annual Meeting, to be held July 6-10, 2009, in Denver, Colorado. The award will consist of a certificate and a cash award of 1000US dollars. The recipient will be expected to present a lecture. SIAM will reimburse the recipient's expenses to attend the meeting and deliver the lecture.

Nominations should be addressed to Professor Howard Elman, Chair, James H. Wilkinson Prize Committee and sent by **1 November 2008**, to J. M. Littleton at littleton@siam.org. Enquiries should be addressed to littleton@siam.org. See also www.siam.org/prizes/nominations.php.

4 Report on the LMS Durham Symposium, 14-24 July 2008

The Durham Symposium on Computational Linear Algebra for Partial Differential Equations brought together some seventy researchers from around the world to foster interaction and discussion on some of the rapidly developing aspects of computational linear algebra as applied to PDE problems. The main objective was to bring together numerical analysts and other mathematicians working in the three closely-related research areas of *optimization*, *saddle point problems*, and *eigenvalues and model reduction* to discuss the many and varied open questions in the area of *PDE optimization*. A novel feature of the symposium was the Industry Day that was held at the end of the first week and specifically focused on application areas.

Six keynote speakers each gave a mini-series of three lectures on one of the highlighted topics. These talks were designed to introduce less experienced members of the audience (and those from different fields) to the necessary background material from linear algebra and PDEs. All six speakers did an excellent job of stimulating discussion—leading to intensive questioning and fruitful discussion at the end of the majority of the lectures!

The keynote speakers on *eigenvalues and model reduction* were Volker Mehrmann (Berlin) and Alastair Spence (Bath). Spence presented state-of-the-art algorithms for computing (a few) eigenvalues of discretized nonlinear PDE problems with the goal of determining the underlying bifurcation structure of some underlying physical model. Mehrmann focussed on nonlinear eigenvalue problems and stressed the importance of finding structured linearizations of the palindromic/symplectic nonlinear eigenvalue problems which often arise in applications. He also surveyed the requirement for model reduction in the simulation, control and optimization of real world processes. Other participants who gave talks related to this topic were Ernst (Freiberg), Freitag (Bath), Miedlar (PhD student, Berlin), Nichols (Reading) and Cliffe (Nottingham).

Valeria Simoncini (Bologna) and Ragnar Winther (Oslo) were the keynote speakers on *saddle point problems*. Simoncini's survey of the latest developments generated heated discussion. Identifying the "optimal solution method" is ultimately application specific, and so is at odds with the "black-box software" approach historically taken by the numerical optimization community. Winther's first two talks concentrated on saddle point problems arising from discretizations of PDEs. His third talk reviewed his seminal work on finite element exterior calculus culminating in the construction of a preconditioner for the Hodge Laplacian. Other talks concerned with the design of effective preconditioners for saddle point problems were given by Benzi (Emory), Kay (Oxford), Elman, Silvester, and Schöberl (Aachen).

Eldad Haber (Emory) gave three talks where he outlined the challenges facing the optimization community if it is to make an impact in the field of PDE optimization. Problems of flow control

and the like have until recently been considered with simple descent algorithms. However, the real need is to combine knowledge from both optimization and PDEs for devising general and effective approaches. One important observation made is that optimization techniques must take account of the (elliptic, parabolic, hyperbolic) character of the underlying PDE if they are to be effective. To set the ball rolling Haber has provided a suite of model PDE optimization problems in MATLAB : <http://www.mathcs.emory.edu/haber/code.html>

Participants were encouraged to use these as a starting point for testing optimization algorithms and preconditioning approaches.

The topic of *PDE Optimization* gave a focus to the Industry Day. The opening talk was given by Matthias Heinkenschloss (Rice), who motivated the topic of PDE constrained optimization problems using industrial applications. Heinkenschloss then proceeded to give a wonderful overview of the design, theory and application of derivative based optimization algorithms for the solution of such problems. Motivated by applications to cardiac electrophysiology, George Biros (Pennsylvania) presented some fast algorithms for solving inverse problems with elliptic and parabolic PDE constraints. Other talks involving the numerical solution of PDE optimization problems were given by Zuhlehnar (Linz), Dollar (RAL), and Kunoth (Paderborn). More general optimization talks were given by Cartis (Edinburgh), Kocvara (Birmingham), Leyffer (Argonne) and Lawless (Reading).

Max Gunzburger (Florida State) gave his three talks on Stochastic PDEs in the second week. The first talk started at an introductory level, “Numerical Methods for Stochastic PDEs for Dummies”, where the huge dimensionality of the associated discrete linear algebra systems was identified as the source of difficulty ultimately constraining the accuracy of solution. The second and third talks covered state-of-the-art approximation methods that radically reduce the dimension of the discrete systems. These include Stochastic Collocation based on Smolyak quadrature, and non-intrusive polynomial chaos methods. Gunzburger also presented numerical results showing that these dimensional reduction techniques make it feasible to solve Stochastic PDE constrained optimization problems. A real breakthrough! Complementary talks discussing linear algebra aspects of discretized Stochastic PDE problems were given by Powell (Manchester) and Ullmann (Freiberg, PhD student).

Video recordings of talks and associated slides in pdf format are also available online, see <http://www.maths.dur.ac.uk/events/Meetings/LMS/2008/CLAPDE/talks.html>

David Silvester (Manchester)

5 Bath/RAL Numerical Analysis Day 2008

The Bath/RAL NA Day is an annual event held alternately at the University of Bath and the Rutherford Appleton Laboratory. This year’s event was the seventh in the series and was held on 23 September in Bath. The day was well attended with substantial delegations from Bath, RAL, Reading and NAG.

There were 3 speakers in the morning session: Marco Marletta (Cardiff), Jonathan Hogg (Edinburgh and RAL) and Ivan Graham (Bath) and three speakers after lunch: Mario Arioli (RAL), Melina Freitag (Bath) and Mike Powell (Cambridge).

Marco Marletta considered numerical methods for eigenvalue problems for PDEs on exterior domains. As a model problem he introduced the Schrödinger equation. Typically the self-adjoint operator associated with the problem has an essential spectrum consisting of continuous bands and discrete eigenvalues in the gaps and possibly the bands as well. An important problem is the numerical calculation of the eigenvalues in the gaps. Marletta outlined alternative approaches and discussed their limitations, focusing then on the domain truncation method that approximates exterior problems by problems on larger and larger finite domains with specially chosen boundaries. This method can be formulated in terms of so-called Dirichlet to Neumann maps. A Dirichlet to Neumann map takes a function on the boundary of a domain to a function on the same boundary by using the input function as a Dirichlet boundary condition, solving a PDE and taking the normal derivative of the solution on the boundary as the output function. Such a map is an analytic function between Sobolev spaces whose poles are the eigenvalues of the self-adjoint operator. Marletta tightened existing theory, showing convergence in the operator norm, locally uniform in the spectral parameter. The new results are such that they can be exploited in numerical methods.

Jonathan Hogg, a PhD student at the University of Edinburgh currently working at RAL, presented

work on a mixed precision sparse solver for symmetric systems. The basic algorithm is a sparse matrix factorisation with partial pivoting. Experiments show that, for large enough systems, a single precision implementation is close to twice as fast as a double precision implementation and requires about half the memory to store the factors. The goal is to obtain double precision accuracy using a single precision factorisation. The standard technique of iterative refinement was shown to work for a large number of test problems. Where the required accuracy is not achieved, a more robust approach based on FGMRES using the single precision factorisation as a preconditioner is generally successful. The presented techniques have been implemented within the HSL software package HSL_MA79.

Ivan Graham presented work on methods for high-contrast elliptic interface problems. His model problem was an elliptic equation with a piecewise constant coefficient function modelling a material with inclusions, i.e., regions of high or low coefficients spread throughout the domain. A standard technique is to construct a grid that is aligned with the boundaries of the inclusions. This is not always easy or possible. The aim is to develop methods that find accurate solutions by discretisation on naive grids. A straightforward regular grid is put on the domain without taking the location of the inclusions into account. Special basis functions are then used to discretise the problem on the naive grid. Coefficient explicit theory shows what these should be like. The multiscale finite element method constructs each basis function as the solution of the original problem restricted to the elements of the grid (a type of subgrid modelling). Boundary conditions have to be chosen for each subproblem and this has to be done in a clever way. The main result presented was a theorem showing convergence with respect to the mesh resolution with the same order as for the constant coefficient case.

Mario Arioli from RAL discussed least squares problems and stopping criteria for the conjugate gradient method for the normal equations. The least squares problem can be interpreted as a statistical problem in which case it corresponds to a Markov-Gauss problem. This perspective suggests different stopping criteria than the ones traditionally used. The resulting theory was illustrated using numerical experiments.

Melina Freitag, a GWR postdoctoral fellow at Bath working closely with the Met Office, presented her work on data assimilation, a technique that has numerical weather forecasting as one of its important applications. Given a background state (such as a previous prediction of the evolution of the system) and a set of observations, the problem is to find a better approximation of the evolution of the state of the system. The updated state can then be used as the initial condition for a new forecast. This approach leads to a large scale optimisation problem. The 3D Var method uses only the information at one point in time. The 4D Var method uses the evolution of the system and observations in a certain time window. This method is closely related to the Kalman filter and extended Kalman filter methods. It was pointed out that 4D Var is essentially the same as Tikhonov regularisation. The methods were illustrated using model problems, specifically the three body problem and a Lorenz system. An interesting idea for future research is to substitute the l_2 -norm regularisation of 4D Var, which smears out shocks, with l_1 -norm regularisation which could provide better shock capturing features.

Mike Powell, an authority on optimisation methods, spoke on the development of NEWUOA, a software package for unconstrained optimisation that does not use derivatives of the objective function. Observing that a quadratic function of n arguments is specified by $O(n^2)$ parameters and thus $O(n^2)$ function evaluations are needed to estimate the shape of the quadratic, one expects that $O(n^2)$ function evaluations are needed to find the optimum of a quadratic function. Experiments show, however, that it is possible to construct methods for which the number of iterations seems to behave like $O(n)$. NEWUOA implements a trust region method. The method starts with a quadratic model with a diagonal Hessian. The model is estimated using interpolation at m points, with typically $m = 2n + 1$. The centre of the trust region is updated whenever a better point is found. Each new function evaluation is used to update the quadratic model. The update is chosen to minimise the change in Hessian of the model. This can be done in an efficient and stable manner by updating an appropriate representation of the inverse of a matrix. The choice of interpolation point to replace at each step was briefly discussed. The methods was shown to be very effective for some hard test problems. The software is available by emailing mjdp@cam.ac.uk.

After a day of excellent presentations, some of the attendants joined the organizers for a meal in the Italian restaurant Aqua in the centre of Bath. Returning home proved to be slightly eventful for some because of an exploding gas canister on a building site near the railway station. Some trains were cancelled and the access to the station was limited for a while, but a reasonable service was reestablished eventually. We hope that everyone made it home without too many problems.

Jan van Lent (Bath)

6 Who's Visiting Whom

Birmingham

Dr Maxim Olshanskii (Moscow State University) is visiting Dr Daniel Loghin between 29/09 and 3/10. His research interests are numerical analysis, multigrid methods, numerical linear algebra with applications to solving partial differential equations and Computational Fluid Dynamics.

Oxford

Dr Martin Lotz (University of Paderborn and City University of Hong Kong), is visiting OUCL from July 2008 to September 2009. He is working with Dr Raphael Hauser on "Geometric Methods and Probabilistic Analysis of Condition Numbers".

Rutherford Appleton Laboratory

Dr Fred Wubs (Groningen University) is visiting Dr Jennifer Scott and the Numerical Analysis Group at RAL between 1 November 2008 and 31 March 2009. He will be working with the Group on the solution of large sparse symmetric indefinite systems of equations.

7 Technical Reports

University of Bath

BICS reports: Available from <http://www.bath.ac.uk/math-sci/bics/preprints/>

- 13/08 Random networks with sublinear preferential attachment: Degree evolutions.
Steffen Dereich and Peter Mrters.
- 12/08 Energy minimizing coarse spaces for two-level Schwarz methods for multiscale PDEs.
J. Van lent, R. Scheichl and I.G. Graham.
- 11/08 The robustness of the emergent scaling property of random RC network models of complex materials. N. J. McCullen, D. P. Almond, C. J. Budd and G. W. Hunt.
- 10/08 Minimal supporting subtrees for the free energy of polymers on disordered trees.
Peter Mrters and Marcel Ortgiese.
- 9/08 Exact modelling of the phases at the triple point of zirconia.
Kai Hormann and Johannes Zimmer.
- 8/08 Gradient flows in asymmetric metric spaces.
Isaac Vikram Chenchiah, Marc Oliver Rieger and Johannes Zimmer.
- 7/08 A Bayesian moving average model for correlated count data.
Duncan Lee, Ruth Salway, Gavin Shaddick and Stephen Walker.
- 6/08 Boundary integral methods in high frequency scattering.
Simon N. Chandler-Wilde and Ivan G. Graham.
- 5/08 Moving mesh generation using the Parabolic Monge-Ampre equation.
C. J. Budd and J. F. Williams.

Brunel University

http://people.brunel.ac.uk/~icsrssi/bicom/tech_rep.html

- BICOM 08/3 S Shaw, MK Warby and JR Whiteman.
Discretization error and modelling error in the context of the rapid inflation of hyperelastic membranes.

University of Cambridge

Reports available from <http://www.damtp.cam.ac.uk/user/na/reports.html>

- NA2008/10 On highly oscillatory problems arising in electronic engineering.
Marissa Condon, Alfredo Deao and Arieh Iserles.
- NA2008/09 Magnus expansions and beyond. Arieh Iserles.
- NA2008/08 Sparse grid modified Fourier series and application to boundary value problems.
Ben Adcock.
- NA2008/07 On modified asymptotic series involving confluent hypergeometric functions.
Alfredo Deao and Nico M. Temme.
- NA2008/06 On the convergence of a wide range of trust region methods for unconstrained optimization.
M.J.D. Powell.
- NA2008/05 The spectral problem for a class of highly oscillatory Fredholm differential equations.
Hermann Brunner, Arieh Iserles and Syvert Nrsett.

Cardiff University

- 07/14 D Rh Gwynllyw and T N Phillips.
The influence of Oldroyd-B and PTT lubricants on moving journal bearing systems.
- 07/15 P. Bollada. Expansion of elastic bodies with application in the bread industry.
- 08/01 F. Bierbrauer, P. C. Bollada and T. N. Phillips.
A consistent reflected image particle approach to the treatment of boundary conditions in smoothed particle hydrodynamics.
- 08/02 P. C. Bollada and T. N. Phillips.
On the formulation of mathematical models for compressible viscoelastic fluids.
- 08/03 R. O. Vargas, O. Manero and T.N. Phillips.
Viscoelastic flow past confined objects using a micro-macro approach.
- 08/04 F. Bierbrauer and T. N. Phillips.
Secondary atomisation: simulation of the droplet break-up in disturbed flow fields.
- 08/05 F. Bierbrauer F and T. N. Phillips.
Modelling spray impingement onto flat, rigid walls using an Eulerian-Lagrangian method.
- 08/06 G. M. Leonenko and T. N. Phillips. On the solution of the Fokker-Planck equation using a high-order reduced basis function approximation.
- 08/07 P. C. Bollada and T. N. Phillips.
A modified deformation field method for integral viscoelastic constitutive equations.
- 08/08 G. M. Leonenko and T. N. Phillips.
Reduced basis function method for solving the 2D Fokker-Planck equation.

University of Edinburgh

Reports available from <http://www.maths.ed.ac.uk/ERGO/preprints.html>

ERGO 08-002 H. Du, P.-J. Chung, J. Gondzio and B. Mulgrew.
Discretization error and modelling error in the context of the rapid inflation of hyperelastic membranes.

University of Manchester

MIMS EPrints from <http://www.manchester.ac.uk/mims/eprints>

- 2008.77: Younes Chahlaoui and Paul Van Dooren (2008).
First/second order transformation system. Tentative proof.
- 2008.74: N Polydorides, E Storteig and W. R. B. Lionheart (2008).
Ocean Current Prediction In Towed Cable Hydrodynamics Under Dynamic Steering.
- 2008.66: Darran Furnival, Howard Elman and Catherine Powell (2008).
H(div) Preconditioning for a Mixed Finite Element Formulation of the Stochastic Diffusion Problem.
- 2008.61: David A. Kay, Philip M. Gresho, David F. Griffiths and David J. Silvester (2008).
Adaptive time-stepping for incompressible flow Part II: Navier-Stokes Equations.
- 2008.60: D. Steven Mackey, Niloufer Mackey, Christian Mehl and Volker Mehrmann (2007).
Numerical methods for palindromic eigenvalue problems: Computing the anti-triangular Schur form. Numerical Linear Algebra with Applications.
- 2008.55: Christopher J. Munro (2007).
Deflating Quadratic Matrix Polynomials. Masters thesis, The University of Manchester.
- 2008.50: Rudiger Borsdorf and Nicholas J. Higham (2008).
A Preconditioned Newton Algorithm for the Nearest Correlation Matrix.
- 2008.49: Rudiger Borsdorf (2007).
A Newton Algorithm for the Nearest Correlation Matrix. Masters thesis, University of Manchester.
- 2008.47: Juan Felipe P. J. Abascal and William R. B. Lionheart (2004).
Rank analysis of the anisotropic inverse conductivity problem. In: International Conference on Electrical Bioimpedance and Electrical Impedance Tomography, 20-24 June 2004, Gdansk, Poland.
- 2008.43: William R. B. Lionheart (2001).
Reconstruction Algorithms for Permittivity and Conductivity Imaging. Proceedings of the 2nd World Congress on Industrial Process Tomography, Hannover, Germany, Wednesday 29th to Friday 31st August 2001. pp. 4-11.
- 2008.40: Timo Betcke, Nicholas J. Higham, Volker Mehrmann, Christian Schröder and Françoise Tisseur (2008).
NLEVP: A Collection of Nonlinear Eigenvalue Problems.
- 2008.35: Ralph Byers, D. Steven Mackey, Volker Mehrmann and Hongguo Xu (2008).
Symplectic, BVD, and Palindromic Approaches to Discrete-Time Control Problems.

University of Oxford

Reports available from <http://web.comlab.ox.ac.uk/oucl/publications/natr/index.html>

- NA-08/12 Householder triangularization of a quasimatrix. L N Trefethen.
- NA-08/11 Piecewise smooth chebfuns. T Driscoll, F Bornemann and L N Trefethen.
- NA-08/10 Optimal solvers for PDE-Constrained Optimization. T Rees, H S Dollar and A J Wathen.
- NA-08/09 A second derivative SQP method with imposed descent. N I M Gould, D P Robinson.
- NA-08/08 A Bramble-Pasciak-like method with applications in optimization.
H S Dollar, N I M Gould, M Stoll, and A J Wathen.
- NA-08/07 Piecewise smooth chebfuns. R Pachn, R Platte and L N Trefethen.
- NA-08/06 GMRES for the differentiation operator. S Olver.
- NA-08/05 A Primal-Dual Augmented Lagrangian. P E Gill, D P Robinson.
- NA-08/04 A Sixth-Order Extension to the MATLAB Package `bvp4c` of J. Kierzenka and L. Shampine. N Hale, D R Moore.

Rutherford Appleton Laboratory

Reports available from <http://www.numerical.rl.ac.uk/reports/reports.html>

- RAL-TR-2008-028 N. I. M. Gould and V. Simoncini
Spectral analysis of saddle point matrices with indefinite leading blocks.
- RAL-TR-2008-027 J. K. Reid and J. A. Scott
Guidelines for the development of HSL software.
- RAL-TR-2008-026 S. Bellavia, C. Cartis, N. I. M. Gould, B. Morini and Ph. L. Toint
Convergence of a regularized Euclidean residual algorithm for nonlinear least-squares.
- RAL-TR-2008-023 J. D. Hogg and J. A. Scott
A fast and robust mixed precision solver for the solution of sparse symmetric linear systems.
- RAL-TR-2008-019 N. I. M. Gould and D. P. Robinson
A second derivative SQP method with imposed descent.
- RAL-TR-2008-018 T. Rees, H. S. Dollar and A. J. Wathen
Optimal solvers for PDE-Constrained Optimization.
- RAL-TR-2008-017 H. S. Dollar, N. I. M. Gould, M. Stoll and A. J. Wathen
A Bramble-Pasciak-like method with applications in optimization.
- RAL-TR-2008-016 J.A. Scott
Scaling and pivoting in an out-of-core sparse direct solver.
- RAL-TR-2008-015 J.V. Ashby and J.K. Reid
Migrating a scientific application from MPI to coarrays.
- RAL-TR-2008-014 I.S. Duff and B. Ucar

On the block triangular form of symmetric matrices.

- RAL-TR-2008-013 P.R. Amestoy, I.S. Duff, D. Ruiz, and B. Ucar
A parallel matrix scaling algorithm.
- RAL-TR-2008-012 M. Arioli and D. Loghin
Discrete interpolation norms with applications.
- RAL-TR-2008-010 Z.-Z. Bai, I. S. Duff and J.-F. Yin
Numerical study on incomplete orthogonal factorization preconditioners.
- RAL-TR-2008-009 I. S. Duff and D. Mijuca
On the efficient solution of mixed finite element equations in geometrically multiscale thermal stress analysis.
- RAL-TR-2008-008 M. Arioli and S. Gratton
Least-squares problems, normal equations, and stopping criteria for the conjugate gradient method.

8 Diary of Seminars (October - December 2008)

BATH Numerical Analysis Seminars: Seminars take place on Fridays at 12:15pm in Department of Mathematical Sciences, Building 1 West, Room 1W3.6. The timetable is available at <http://www.maths.bath.ac.uk/~jvl20/na-seminars>

BATH BICS series: Seminars take place at 1:15pm in Department of Mathematical Sciences, Building 1 West, Room 1W3.6. A timetable is available at <http://www.bath.ac.uk/math-sci/bics/seminars/>

BATH CNM Seminars: Seminars take place on Tuesdays at 1:15pm in the Department of Mathematical Sciences, Building 1 West, Room 1W3.6. The timetable is available at <http://www.bath.ac.uk/cnm/>

BATH CNM series: Seminars take place on Tuesdays at 1:15pm in the Department of Mathematical Sciences, Building 1 West, Room 1W3.6. The timetable is available at <http://www.bath.ac.uk/cnm/>

BIRMINGHAM : The Optimisation and Numerical Analysis seminar at Birmingham run on Thursdays, between 12-1pm in Arts Lecture Room 6, Edgbaston Campus at the University of Birmingham. The programme can be found at <http://web.mat.bham.ac.uk/loghin/onaseminars.html>

BRUNEL : Two seminar series are held in the Department of Mathematical Sciences, John-Crank Building, Room M128. The Applied Mathematics Research Seminars take place on Mondays at 14:00, and the Seminars on Mathematical Physics and Random Matrices are held on Tuesdays at 16:00. More details are available at <http://www.brunel.ac.uk/about/acad/siscm/math/events>

CARDIFF : Seminars take place on Mondays at 3pm in School of Mathematics room M/2.06. Contact: Tim Phillips (phillipstn@cardiff.ac.uk).

CAMBRIDGE : There are three relevant seminar series in Cambridge which are held in MR14, Pavilion F, Centre for Mathematical Sciences: Applied and Computational Analysis Seminars (up-to-date details at <http://www.damtp.cam.ac.uk/user/na/ACA/>), Numerical Analysis Seminars (up-to-date details at <http://www.damtp.cam.ac.uk/user/na/seminars.html>), and ACA Graduate Seminars (up-to-date details at <http://www.damtp.cam.ac.uk/user/na/GradSeminar.html>).

EDINBURGH : The Edinburgh Research Group in Optimization (ERGO) runs seminars on Optimization and Numerical Analysis. Unless stated otherwise, seminars are held at 3.30pm in Room 6206 of the James Clerk Maxwell Building. More details are available from:

<http://www.maths.ed.ac.uk/ERGO/Seminars.html>

MANCHESTER : Numerical Analysis and Scientific Computing Seminars 2007/08 The seminars are held in the in the Alan Turing Building, Frank Adams Room 1, at 3pm. For more details and abstracts, see <http://www.mims.manchester.ac.uk/events/seminars/numerical-analysis.php>

OXFORD : Seminars take place on Thursdays at 2pm in the Lecture Theatre of Oxford University Computing Laboratory, Wolfson Building, Parks Road. A timetable and abstracts are available from <http://web.comlab.ox.ac.uk/oucl/news/>

RAL : Seminars are held in the Atlas Centre, Rutherford Appleton Laboratory and start at 2pm.
Contact: s.dollar@rl.ac.uk

READING : Seminars take place on Fridays promptly at 3pm in room 113 of the Mathematics Department. External audiences are advised to contact Brigitte Calderon on 0118 378 5002 or email b.calderon@reading.ac.uk to confirm the programme before attending.

OCTOBER 2008

OCTOBER 1 : EDINBURGH. Simon Tett (Edinburgh). Introduction to climate modelling.

OCTOBER 2 : BIRMINGHAM. Gemayqzel Bouza (Madrid and Havana). Title TBA.

OCTOBER 9 : BIRMINGHAM. Juan-Enrique Martinez Legaz (Barcelona). Monotone operators: convex representations and surjectivity theorems.

OCTOBER 9 : OXFORD. Michael Floater (Oslo). Barycentric coordinates and transfinite interpolation.

OCTOBER 10 : READING. Peter Grindrod (Reading). Fractals, Flows and IFS over Banach Spaces: Long Time Behaviour of Hybrid Parabolic PDEs

OCTOBER 10 : MANCHESTER. John Barrett (Imperial College). Parametric Approximation of Geometric Evolution Equations.

OCTOBER 13 : BATH. Mike Finnis (Imperial College). Calculation of the equilibrium concentration of point defects in alumina.

OCTOBER 15 : EDINBURGH. Alexander McNeil (Heriot-Watt University). Title TBA.

OCTOBER 16 : BIRMINGHAM. Marco Lopez (Alicante). Title TBA.

OCTOBER 16 : OXFORD. David Mayers (Oxford). Title TBA.

OCTOBER 17 : READING. Frank Bauer (Johannes Kepler University of Linz) Parallel MRI - Quality and Speed, a contradiction?

OCTOBER 20 : BATH. Joshy Eashaw (Bath). Households forming macroeconomic expectations: the case of spatial learning.

OCTOBER 22 : BATH. 4th Numerical Analysis Postgraduate Seminar Day.
See <http://www.maths.bath.ac.uk/~mamamf/pgnaday.html>

OCTOBER 23 : CAMBRIDGE. Darryl Holm (Imperial College). Title TBA.

OCTOBER 23 : RAL. Marc Baboulin (Coimbra). Some issues in dense linear algebra algorithms for multicore and new architectures.

OCTOBER 24 : MANCHESTER. Erik Burman (Sussex). Title TBA

OCTOBER 24 : READING. Roland Potthast (Reading). Simulation and Inversion for Cognitive Neurodynamics.

OCTOBER 27 : BATH. Roland Potthast (Reading). Title TBA

OCTOBER 30 : EDINBURGH. Raphael Hauser (Oxford). Robust portfolio optimization with structured uncertainty sets.

OCTOBER 31 : READING. Qingping Zou (Plymouth). Title TBA

NOVEMBER 2008

NOVEMBER 3 : BATH. Peter Allen (Cranfield). Title TBA

NOVEMBER 6 : CAMBRIDGE. Bryce McLeod (Oxford). Title TBA.

NOVEMBER 6 : BIRMINGHAM. Emmanuil Georgoulis (Leicester). Discontinuous Galerkin methods for convection-diffusion-reaction problems: a survey and some recent results.

NOVEMBER 6 : OXFORD. Divakar Viswanath (Michigan). Asymptotics and complex singularities of the Lorenz attractor.

NOVEMBER 7 : MANCHESTER. Michal Kocvara (Birmingham). Title TBA

NOVEMBER 7 : READING. Yulii Shikmurzaev (Birmingham). Capillary Flows with Forming Interfaces: Paradoxes of Classical Fluid Mechanics.

NOVEMBER 10 : BATH. Kirill Cherednichenko (Cardiff). Title TBA

NOVEMBER 12 : EDINBURGH. Jonathan Hogg (RAL and Edinburgh). Mixed precision solution of linear systems.

NOVEMBER 13 : BIRMINGHAM. Coralia Cartis (Edinburgh). Title TBA.

NOVEMBER 13 : OXFORD. Frederic Nataf (Paris VI). Optimal domain decomposition methods (Neumann-Neumann or FETI types) for systems of PDEs.

NOVEMBER 17 : BATH. Tim Ibell (Bath). Realistic structural assessment and strengthening design approaches for our buildings.

NOVEMBER 19 : EDINBURGH. Angela Mihai (Cambridge). Title TBA.

NOVEMBER 20 : OXFORD. Soren Bartels (Bonn). Approximation of harmonic maps and wave maps.

NOVEMBER 20 : BIRMINGHAM. Françoise Tisseur (Manchester). How to Detect Definite Hermitian Pairs.

NOVEMBER 21 : CAMBRIDGE. Alfio Quarteroni (EPFL). Title TBA (this is a joint seminar with fluid dynamics, at 4pm, MR2, Central Core, CMS).

NOVEMBER 21 : MANCHESTER. Angela Mihai (Cambridge). Title TBA

NOVEMBER 21 : READING. Mike Kirby (University of Utah, visiting Imperial College). The material point method.

NOVEMBER 24 : BATH. Stephen Coombes (Nottingham). Title TBA

NOVEMBER 25 : CARDIFF. Sergei Chernyshenko (Imperial). Streaks and stripes: applying linear equations to nonlinear turbulence.

NOVEMBER 26 : EDINBURGH. Michal Kocvara (Birmingham). Title TBA.

NOVEMBER 27 : CAMBRIDGE. Laurent Desvillettes (ENS Cachan). Title TBA

NOVEMBER 27 : RAL. Alicia Kim (Bath). Topology Optimisation: Achievements and Challenges.

NOVEMBER 28 : READING. Marcus Tindall (Reading). Intracellular signalling in bacterial chemotaxis: From reaction diffusion to fractional reaction diffusion equations.

DECEMBER 2008

DECEMBER 1 : BATH. David Balding (Imperial College). Analysis of population structure from canine pedigrees.

DECEMBER 2 : CARDIFF. Jonathan Evans (Bath). Re-entrant corner behaviour of some common viscoelastic fluids.

DECEMBER 4 : OXFORD. Jonathan Hogg (RAL). Cholesky factorizations for multi-core systems.

DECEMBER 5 : MANCHESTER. Coralia Cartis (Edinburgh). Title TBA

DECEMBER 8 : BATH. Eve Middleton-Kelly (LSE). Title TBA

DECEMBER 12 : READING. Fred Wubs (Groningen). Preconditioning for an implicit thermohaline circulation model.

DECEMBER 19 : MANCHESTER. Jitse Niesen (Leeds). Title TBA

9 Forthcoming Meetings and Conferences**OCTOBER 2008****4th MIDNAG meeting, October 1.**

Birmingham. <http://www.mat.bham.ac.uk/research/applied/MIDNAG/>

International Conference on Applied Mathematics and Approximation Theory 2008, October 11-13.

University of Memphis, USA. <http://www.mscl.memphis.edu/AMAT2008/>

International Workshop on Numerical Analysis and Scientific Computing, October 13-17.

Rostov-on-Don, Russia. <http://conf.rsu.ru/nascom08/>

Computer Aspects of Numerical Algorithms (CANA'08), October 20-22.

Wisla, Poland. <http://www.cana.imcsit.org>

Ninth European Multigrid Conference, in Honour of Wolfgang Hackbusch's sixtieth birthday, October 20-23.

Bad Herrenalb, Germany. <http://www.techsim.info>

Symposium in Honour of Wolfgang Hackbusch's sixtieth birthday, October 24.

Bad Herrenalb, Germany. <http://www.techsim.info>

Model reduction for circuit simulation, October 30-31

University of Hamburg, Germany. <http://www.math.uni-hamburg.de/spag/zms/syrene/>

DECEMBER 2008**Third International Conference on Scientific Computing and Partial Differential Equations, December 8-12.**

Hong Kong Baptist University. <http://www.math.hkbu.edu.hk/SCPDE08/>

Numerical Analysis and Optimization (JANO9), December 17-19.

Mohammedia, Morocco. <http://www.fstm.ac.ma/jano9>

15th IEEE International Conference on High Performance Computing (HiPC 2008), December 17-20.

Bangalore, India. <http://www.hipc.org>

JANUARY 2009

Finite Element Methods in Engineering and Science, January 5-9.

Lake Tahoe, USA. http://servac.math.utep.edu/femtec_2008/home

Annual Meeting UK and Republic of Ireland SIAM Section, January 9.

Limerick, Ireland. <http://www.numerical.rl.ac.uk/people/hsd/ukiesiam/>

Annual GAMM Seminar, January 22-24.

Leipzig, Germany. <http://www.mis.mpg.de/scicomp/gamm25/index.html>

MARCH 2009**SIAM Conference on Computational Science and Engineering (CSE09), March 2-6.**

Miami, Florida. <http://www.siam.org/meetings/cse09/>

APRIL 2009**Annual European Rheology Conference (AERC), 15-17 April.**

Cardiff. <http://www.rheology-esr.org/AERC/2009>

MAY 2009**SIAM Conference on Applications of Dynamical Systems (DS09), May 17-21.**

Snowbird, Utah. <http://www.siam.org/meetings/ds09/>

Numerical Analysis and Scientific Computation with Applications, May 18-22.

Agadir, Morocco. <http://www-lmpa.univ-littoral.fr/NASCA09/>

International Conference on Scientific Computation and Differential Equations (SciCADE09), May 25-29.

Beijing, China. <http://lsec.cc.ac.cn/~scade09/>

JUNE 2009**Large-Scale Scientific Computations (LSSC), June 4-6.**

Sozopol, Bulgaria <http://parallel.bas.bg/Conferences/SciCom09.html>

23rd Biennial Conference on Numerical Analysis, June 23-26.

Strathclyde University, Glasgow. <http://www.maths.strath.ac.uk/naconf>

14th Leslie Fox Prize meeting, June 29.

University of Warwick.

JULY 2009**Sparse Matrices for Scientific Computation: In Honour of John Reid's 70th Birthday, July 15-16.**

Abingdon, Oxfordshire. <http://www.numerical.rl.ac.uk/people/hsd/jkr/>

AUGUST 2009**20th International Symposium of Mathematical Programming (ISMP), August 23-29.**

Chicago, Illinois. <http://www.ismp2009.org/>

OCTOBER 2009**SIAM Conference on Applied Linear Algebra (LA09), October 26-29.**

Seaside, California. <http://www.siam.org/meetings/calendar.php>

SIAM Combinatorial Scientific Computing (CSC09), October 29-31.

Seaside, California <http://www.siam.org/meetings/calendar.php>

10 Highlighted Conferences and Workshops

Computational Methods for Non-Newtonian Flows (Fourth MIDNAG meeting)

The 4th MIDNAG meeting is scheduled to take place at the University of Birmingham on October 1st. For more information please visit <http://www.mat.bham.ac.uk/research/applied/MIDNAG/>

The speakers will be:

- Tim Phillips (Cardiff). Macroscopic and micro/macro methods for viscoelastic flows.
- Oliver Harlen (Leeds). TBA
- Maxim Olshanskii (Moscow State). Finite-difference methods and iterative solvers for Bingham flows.
- Erik Burman (Sussex). TBA

Other MIDNAG meetings this year:

- Wednesday 19 November, University of Leicester. Analytical and Computational Techniques for 4th Order PDE
- Wednesday 3 December, University of Nottingham. TBA

Annual European Rheology Conference (AERC) 2009 Cardiff, 15-17 April 2009

AERC 2009 is being organized by the Institute of Non-Newtonian Fluid Mechanics (Wales) and the British Society of Rheology. The aim of AERC 2009 is to contribute to the advancement of Rheology by bringing together interested researchers from Europe and the rest of the world, and bridging traditional themes with modern trends.

Following the tradition of previous European Rheology meetings, AERC 2009 will be a three day conference split into symposia that reflect mainstream or emerging areas of Rheology. There will be minisymposia on blends, copolymers and nanocomposites; process modelling; rheometry and beyond; advanced experimental methods; interfacial phenomena, surfactants and foams; suspensions and colloids; viscoplasticity, solids rheology; biopolymers, biorheology and food rheology; constitutive modelling; non-Newtonian fluid mechanics; computational modelling; flow-induced phase transitions and instabilities; industrial rheology and processing.

Cardiff, the capital city of Wales, is home to many national institutions including the National Museum of Wales and the much-admired Millennium Stadium. The city centre skyline is testimony to its heritage and ambition, with landmark buildings ranging from the ornate civic centre to the historic Cardiff Castle. Cardiff is well established as Europe's Youngest Capital but its history dates back more than 2000 years to the Romans. It was once one of the busiest ports in the world, exporting the coal which fuelled the industrial revolution.

Plenary Speakers:

- Christian Bailly (Universite catholique de Louvain, Belgium)
- Jae Hyun (Korea University, Korea)
- Gareth McKinley (Massachusetts Institute of Technology, USA)

In addition, the meeting will include the 2009 Weissenberg Award Lecture and the 2009 BSR Gold Medal Lecture.

For more information see: <http://www.rheology-esr.org/AERC/2009>

11 Networks

Leverhulme International Research Network: Numerical and Analytical solution of Stochastic Delay Equations

I am pleased to announce the formation of a new international research network, based at the University of Chester, UK and funded by the Leverhulme Trust on the Numerical and Analytical solution of Stochastic Delay Equations.

The network will hold regular workshop meetings. The first workshop will be held in Chester from 3rd-7th November 2008. Details of the programme, feature speakers, registration and accommodation appear in the meetings section of our website at <http://www.chester.ac.uk/math/conferences/meeting08.html> We are also inviting proposals for contributed talks. For further scientific information, please email me or for more general enquiries or if you would like to join our mailing list for news of future events, email Nicola.Williams@chester.ac.uk

Neville Ford (njford@chester.ac.uk), Director of the Research Network.

Matrix and Operator Pencils

Cardiff is coordinating a new EPSRC Network on Matrix and Operator Pencils over the next 3 years. Marco Marletta (MarlettaM@cardiff.ac.uk) is the PI on this grant. The network nodes are:

- Bath
- Birmingham + Manchester
- Cardiff + Liverpool
- Heriot-Watt + Strathclyde
- KCL + UCL
- Lancaster
- Nottingham
- Reading

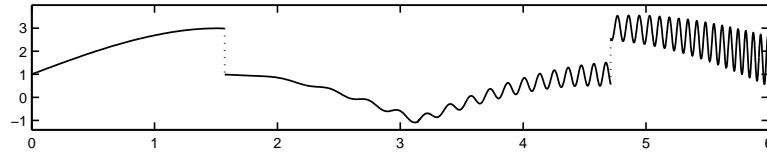
The Scientific Committee comprises Brian Davies, Nick Higham, John McWhirter, Seamus Garvey and Alastair Spence.

12 Software News

CHEBFUN AND CHEBOP

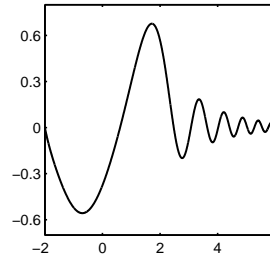
“Chebyshev technology”, the use of Chebyshev series and interpolants for numerical computation, saw much of its early development in the 1950s and 1960s in England. Some of the contributions of those good old days include Lanczos’s *Applied Analysis* with his Chebyshev tau method (Dublin, 1956), Clenshaw and Curtis’s Chebyshev quadrature formula (NPL, 1960), Good’s colleague matrices for Chebyshev zero-finding (NPL, 1961), Fox and Parker’s survey of early steps toward Chebyshev spectral methods (Oxford, 1968) and Salzer’s barycentric formula for interpolation in Chebyshev points (New York, 1972). Also important were Elliott, Mason, Wright . . .

It all sounds a bit old-fashioned. It shouldn’t, though, for these methods are potentially even more important with today’s computers than they were back then. Many readers of this newsletter may have attended a talk by me or my collaborators on the chebfun system in object-oriented MATLAB, which puts these ideas into action in a way Clenshaw hardly dreamt of. If you execute `f=chebfun('2*abs(sin(x))+sign(cos(x))+.005*x.^3.*sin(x.^3)',[0 6])`, for example, the system works out in 1/4 second that this function can be represented to machine precision by a concatenation of four polynomial pieces of degrees 28, 48, 79 and 99:



Once you've got the chebfun, you can find its integral with `sum(f)`, maximum with `max(f)`, roots with `roots(f)`, point values with (say) `f(0:6)` and so on, all at great speed to roughly machine precision. And you can carry out further computations like `f.^2` or `exp(f)` with "symbolic feel and numerical speed".

The chebop system takes the next step and overloads linear operators within the same framework via lazy evaluation of spectral differentiation matrices (far from obvious!—no space to explain here). Thus for example if we execute the commands `[d,x]=domain(-2,6)`, `D=diff(d)`, `X=diag(x.^3)`, `L=D^2+D+X`, `L.bc='dirichlet'`, `u=L\1`, in about 0.1 secs. we get the solution to $u'' + u' + x^3u = 1$ with zero boundary conditions on $[-2, 6]$ (right).



We hope that chebfuns and chebops will prove a step towards computing as easily with functions in the 21st century as we learnt to do with numbers in the 20th. To find out more, have a look at www.comlab.ox.ac.uk/chebfun/, and please get in touch if you have an application you'd like to explore together. My chebfun teammates are Toby Driscoll, Ricardo Pachón and Rodrigo Platte. Thanks also to Zachary Battles, Folkmar Bornemann and the EPSRC.

Lloyd N. Trefethen, Oxford University Computing Laboratory (Nick.Trefethen@comlab.ox.ac.uk)

NAG

Because I am more closely associated with the library side of NAG's activities, these articles tend to have a natural bias in that direction. To try and redress this balance, I shall describe one of the essential tools we use in our library preparation - the NAG Fortran compiler - and draw attention to the recent release of it on the PC, as part of an integrated development environment called Fortran Builder.

Our Fortran libraries must run correctly on a range of machines and so it is imperative that our source code be standard. Only then can we expect our code to be supported and interpreted in the same way by a range of Fortran compilers. The NAG compiler is an excellent tool for highlighting non-standard code. This is only to be expected as its principal author, Malcolm Cohen, helped define those standards, and is uniquely placed to understand and interpret them.

NAG routines must also be robust during execution. This means that our test programs must be augmented by a compiler that is capable of taking a strong view during execution of any 'loose' programming. The compiler has unsurpassed runtime error detection, with clear, understandable, messages indicating where and why the code is deficient. For example, it is easy to forget to initialise a variable before usage. Sometimes an assumption is made that a variable will take an initial value of 0. Often this is true, but this cannot be guaranteed under all circumstances, especially if the environment changes for some reason. NAG found a handful of compilers that were capable of detecting uninitialised real and double precision quantities, but found fewer capable of reporting on uninitialised integer quantities. The NAG compiler detects and reports upon uninitialised variables of all types.

The compiler goes far beyond that of course: array subscripts, null pointers, procedure calls, dangling pointers are all thoroughly checked. It is also possible to trace memory allocation.

The NAG compiler supports several Fortran 2003 additions: allocatable components, IEEE arithmetic and several object oriented programming features. NAG continues to develop the compiler and to include more object-oriented features especially; imminent are cloning, type-bound procedure and generic procedures and operators.

For checking purposes alone we would recommend the compiler; even if you have a different compiler it is always useful to have more than one compiler to validate your code.

Now PC users have the opportunity to use the compiler from Fortran Builder. It enables the compiler to be used easily and painlessly.

The IDE is distributed with additional features. It includes two very useful tools: a Fortran 77 to Fortran 95 converter and a formatting tool for Fortran 90/95 programs. Fortran Builder is integrated very closely with the NAG library and LAPACK. For example, the user may create a NAG Library project. This will copy the corresponding NAG example program for the user to adapt for the his or her specific problem. Of course, the project will have all the relevant linker and compiler flags set to use the associated NAG DLL library.

More details on Fortran Builder are available from our web site at:
<http://www.nag.co.uk/nagware/np/fortranbuilder.asp>

David Sayers (David.Sayers@nag.ac.uk)

HPC Training Available for UK Researchers

NAG is pleased to announce that we are running free HPC training for UK researchers.

NAG provides Computational Science and Engineering (CSE) support for HECToR, the UK Supercomputing Service. You are eligible for training, for which there is no charge, if you are a HECToR user or your work is covered by the remit of either EPSRC, BBSRC or NERC. We provide a regular schedule of courses that cover general HPC topics, such as MPI and OpenMP, as well material specific to HECToR. We can also provide training tailored to your specific requirements and deliver courses at your institution.

For further information and our current training schedule please see:

<http://www.hector.ac.uk/support/cse/schedule/>

A full list of available courses and contact details are here:

<http://www.hector.ac.uk/support/cse/schedule/courselist>

For more information about NAG, HECToR and the CSE service please see the following links:

<http://www.nag.co.uk>

<http://www.hector.ac.uk/>

<http://www.hector.ac.uk/support/cse/>

13 PhD Theses

Open University

Masoud Saravi. Numerical Solution of Linear Ordinary Differential Equations and Differential-Algebraic Equations by Spectral Methods.

Cardiff University

Yu Zheng. Numerical simulation of droplet deformation using spectral element methods. December 2007.

Alison Palmer. Linear stability analysis of plane Poiseuille flow of viscoelastic fluids. June 2008.

University of Bath

Stefano Gianni. Convergence of adaptive FEM for elliptic eigenvalue problems with applications to photonic crystals.

Bruce Boutelje. Approximation of the inertial manifold by linear multistep methods.

14 Recent Appointments

University of Dundee

Prof Ping Lin, Professor of Numerical Analysis (PDEs). See <http://www.maths.dundee.ac.uk/~plin/>

15 Vacant positions and studentships

Research positions are available at CERFACS to work in the Parallel Algorithms Team led by Iain Duff. Positions are now available as a postdoc or senior position starting at a date to be agreed with the successful candidates. The level of the appointments will depend on experience but you should state in the application which level you feel to be appropriate.

The Parallel Algorithms Team is looking for a bright, motivated person with a good research record and the ability to supervise research projects and students. The applicant would be expected to join existing projects in numerical optimization and linear algebra as well as showing initiative in pursuing new research directions. Applications in the areas of massively parallel algorithms and/or robust optimization for problems with uncertain data are preferred.

Additional benefits of the position include a gross salary in the range 2,800 to 3,000 euros per month, excellent travel support, opportunities for supplementary income from teaching or consultancy, access to state-of-the-art computational facilities (high-performance workstations and both SMP/MPP parallel architectures, including our in-house IBM BG/L computer with 4096 cores). A particular strength of CERFACS is its access to real-life applications through strong and well developed academic/industrial collaborations within a very active research program in advanced scientific computing.

Relevant information on the application procedure can be found at <http://www.cerfacs.fr/Admin/rules.html> For detailed information about the Parallel Algorithms Project at CERFACS see <http://www.cerfacs.fr/algor>

Applications should be sent before October 15, 2008 to Xavier Vasseur (vasseur@cerfacs.fr)

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A modified Newton method for solving non-symmetric algebraic Riccati equations arising in transport theory.

225–244 Rommel Bustinza, Gabriel N. Gatica, and Francisco-Javier Sayas.

On the coupling of local discontinuous Galerkin and boundary element methods for non-linear exterior transmission problems.

245–273 Paul Houston, Endre Suli, and Thomas P. Wihler.

A posteriori error analysis of hp-version discontinuous Galerkin finite-element methods for second-order quasi-linear elliptic PDEs.

274–291 Johannes Schropp.

Projected RungeKutta methods for index 3 differentialalgebraic equations near equilibria, periodic orbits and attracting sets.

292–330 John W. Barrett, Harald Garcke, and Robert Nurnberg.

Numerical approximation of anisotropic geometric evolution equations in the plane.

331–353 Serge Nicaise, Katharina Witowski, and Barbara I. Wohlmuth.

An a posteriori error estimator for the Lam equation based on equilibrated fluxes.

354–381 Rob Stevenson and Manuel Werner.

Computation of differential operators in aggregated wavelet frame coordinates.

382–421 Stefano Berrone and Endre Suli.

Two-sided a posteriori error bounds for incompressible quasi-Newtonian flows.

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423–439 Carsten Carstensen.

Convergence of an adaptive FEM for a class of degenerate convex minimization problems.

440–468 Marcus J. Grote, Anna Schneebeli, and Dominik Schtzau.

Interior penalty discontinuous Galerkin method for Maxwell’s equations: optimal L2-norm error estimates.

469–495 Abdallah Bradji and Raphale Herbin.

Discretization of coupled heat and electrical diffusion problems by finite-element and finite-volume methods.

496–521 Vit Dolejsi, Miloslav Feistauer, Vaclav Kucera, and Veronika Sobotikova.

An optimal $L^\infty(L^2)$ -error estimate for the discontinuous Galerkin approximation of a nonlinear non-stationary convectiondiffusion problem.

522–551 Melina A. Freitag and Alastair Spence.

A tuned preconditioner for inexact inverse iteration applied to Hermitian eigenvalue problems.

552–579 Daniele Marazzina.

Stability properties of discontinuous Galerkin methods for 2D elliptic problems.

580–597 Weiwei Sun and Jiming Wu.

Interpolatory quadrature rules for Hadamard finite-part integrals and their superconvergence.

598–618 Michele Benzi and Daniele Bertaccini.

Block preconditioning of real-valued iterative algorithms for complex linear systems.

619–646 Stefano Micheletti, Simona Perotto, and Marco Verani.

Uzawa-based adaptive methods for linear output functionals.

For further details see: www.imanum.oupjournals.org

17 New books

Numerical Methods for Evolutionary Differential Equations, by Uri M. Ascher

Methods for the numerical simulation of dynamic mathematical models have been the focus of intensive research for well over 60 years, and the demand for better and more efficient methods has grown as the range of applications has increased. This textbook develops, analyzes, and applies numerical methods for evolutionary, or time-dependent, differential problems, bridging theory and practice by developing algorithms, concepts, and analysis from basic principles.

This textbook is suitable for researchers and graduate students from a variety of fields including computer science, applied mathematics, physics, earth and ocean sciences, and various engineering disciplines.

“This book achieves the allegedly impossible: it blends informality and rigour, making scientific computing exciting and intellectually honest.”

- Arieh Iserles, University of Cambridge.

Discontinuous Galerkin Methods for Solving Elliptic and Parabolic Equations: Theory and Implementation, by Batrice Riviere

This book covers both theory and computation as it focuses on three DG methods which are variations of interior penalty methods. The author provides the basic tools for analysis and discusses coding issues, including data structure, construction of local matrices, and assembling of the global matrix. Computational examples and applications to important engineering problems are also included.

Appendices contain proofs and MATLAB code for one-dimensional problems for elliptic equations and routines written in C that correspond to algorithms for the implementation of DG methods in two or three dimensions.

Intended for numerical analysts, computational and applied mathematicians, and engineers, the book is also appropriate for graduate courses in finite element methods, numerical methods for partial differential equations, numerical analysis, and scientific computing.

Both books are published by SIAM; see www.siam.org/books for further details.

18 Postgraduate Courses

University of Bath

MSc in Mathematical Sciences

Study full time for one year (12 months) or part time for two years to obtain a Masters Degree in Mathematical Sciences. A broad range of units is available in Pure and Applied Mathematics, Probability and Statistics.

Requirements: First or Upper Second Class Honours Degree in Mathematics, or equivalent. Applications from appropriately qualified overseas students are strongly encouraged.

See <http://www.bath.ac.uk/math-sci/postgraduate/taught/msc-math-sci/>

MSc in Mathematical Biology

The MSc will combine taught core units in mathematics, biology and biochemistry with training in research methods and an individual project.

Students will be members of the Centre for Mathematical Biology, taught and supervised jointly by staff in the Department of Mathematical Sciences and the Department of Biology and Biochemistry. Both departments have strong research portfolios and have demonstrated excellence in teaching over many years.

The MSc is a one year full time programme. It can be used as the first year of an Integrated PhD or as a component of the Graduate School provision for PhD students in mathematical biology.

Fully funded studentships are available to suitably qualified individuals. These have been made available by the BBSRC and the University of Bath.

See <http://www.bath.ac.uk/cmb/msc/>

MSc in Modern Application of Mathematics

Study full time for one year to obtain an MSc degree in Modern Applications of Mathematics at the Department of Mathematical Sciences, University of Bath. (RAE grade 5* for research, QAA grade 24/24 for teaching quality.) This programme is suitable for anyone interested in using mathematics in industry. There are EPSRC Studentships for highly qualified UK and EU applicants only. Applications from appropriately qualified overseas students are strongly encouraged. Financial support is available to pay tuition fees for selected EU applicants. Information on scholarships for study in the UK is available from British Council Scholars. Information on potential funding for students from commonwealth countries is also available from the Association of Commonwealth Universities.

- Learn the latest techniques in applied mathematics and scientific computing
- Examine case studies drawn from industrial problems
- Undertake a supervised project with an optional industrial placement
- Modules in interdisciplinary subjects and key skills
- Individualised study programme

See <http://www.bath.ac.uk/math-sci/postgraduate/taught/msc-modern-app/>

The list of available graduate level courses is available from <http://www.bath.ac.uk/math-sci/postgraduate/research/graduate-school/>

University of Birmingham

The School of Mathematics offers a twelve-month MPhil course in Mathematics and an MSc in Mathematical Finance, which is run jointly with the Department of Economics. In addition, the School offers a standard three-year PhD programme. The MPhil is an ideal preparation for entry into the PhD programme.

More details are available at <http://www.mat.bham.ac.uk/Postgraduate/mphil.htm>

Cardiff University

MSc in Computing in the Physical Sciences

The aim of this course is to offer knowledge and expertise for the cross-disciplinary field of scientific computing, preparing graduates for careers in the development of computer models for industrial or academic applications. The course caters for a range of backgrounds by offering introductory material on either computing and mathematics or the physical sciences. Options allow specialisation in Mathematics and Computing or Chemistry and the Physical Sciences. Part-funded studentships are available which cover fees and make a contribution to living expenses for UK-resident EU citizens. The course is taught jointly by the schools of Chemistry, Mathematics and Computer Science. Special Features of this course include hands-on experience of mathematical programming and atomistic chemical simulation software packages; in-depth treatment of the mathematical basis of simulation and its implementation from specialists research-active in the field; and transferable skills of programming and algorithm design.

The course is suitable for graduates in Mathematics, Computing, Chemistry, Physics or related disciplines: e.g. engineering, Pharmacy and Biochemistry. Applicants should have a First or Second Class UK Honours degree, or equivalent. Applicants whose first language is not English will be required to pass either IELTS or TOEFL exams. Contact Name: Dr James Platts (Tel: +44(0)2920874950, Email: platts@cardiff.ac.uk)

For further details see <http://courses.cardiff.ac.uk/Postgraduate/course/detail/952.html>

University of Edinburgh

The Operations Research Group at the University of Edinburgh is offering a one-year MSc programme in Operations Research that has been successfully running since 2002. The current intake is 55 students, and applications for entry in 2009 are already being accepted. For more information and how to apply, please see www.maths.ed.ac.uk/ormsc/

University of Greenwich

MSc Applied Mathematical Modelling and Scientific Computing (AMMSC).

This Masters programme is run by the Department of Mathematical Sciences at Greenwich, within the School of Computing and Mathematical Sciences (ranked 10th in the 2007 UK departmental ranking). (<http://www.timesonline.co.uk/section/0,,6734,00.html>), The MSc is taught by members of the Centre for Numerical Modelling and Process Analysis, an award winning research group.

The programme aims to train and equip Honours graduates in engineering, science or mathematics and suitably qualified professionals, with the skills required to understand, and use, applied mathematical modelling techniques and scientific Computing technologies in industry. Emphasis is on modelling phenomena governed by the physics of fluid flow, heat transfer, electromagnetics and solid mechanics using CFD, FEA and other software tools. Details of available modules can be found at: <http://ammisc.gre.ac.uk>

CTA (Collaborative Training Awards): Up to eight EPSRC CTA studentships are allocated to this MSc programme to the best qualified candidates who are classified as UK residents. There are two student intakes per annum, in October and January.

Further details of the programme, applications, enquiries should reach cmsinfo@gre.ac.uk (Mrs. Marilyn Nichols) or cse@gre.ac.uk

Heriot-Watt University

We offer a MSc/Diploma in Computational Mathematics in mathematics at Heriot-Watt University. This is a new postgraduate course to provide students with a clear understanding of the main issues in performing and analysing scientific computations.

This is linked to the Applied Mathematical Sciences Graduate Programme which provides transferable,

modern mathematical and numerical skills geared to careers in both research and industry. To achieve this we offer a solid theoretical and practical foundation through a broad range of modules.

These courses are available as a 1 year full-time MSc/Diploma as well as on a part-time basis. We expect some funding to be available for entry in 2009 through SAAS for suitable students.

Further details maybe found at <http://www.ma.hw.ac.uk/mscapmasc/>

Enquiries should be addressed to :

Lisa Keyes, Department of Mathematics,

Heriot-Watt, Edinburgh, EH14 4AS, UK.

Tel : 0131 451 3221. Email : amase@ma.hw.ac.uk

University of Liverpool

Applications are invited for the EPSRC DTA awards (any time before September) and several other PhD vacancies associated with the Department of Mathematical Sciences at the University of Liverpool. Starting in September 2008, the Department will continue running an MSc in Mathematical Sciences that provides training in mathematics with options to specialise in any of the subjects at the project stage. For further details, see http://www.liv.ac.uk/math/Prosp_PG/ and enquiries may be addressed to Ms Shirley Farrell (safrell@liverpool.ac.uk).

University of Manchester

The Schools of Mathematics and Computer Science at the University of Manchester jointly run an MSc in Mathematics and Computational Science that provides training in applied mathematics, numerical analysis, and computational science. It is suitable for students wishing to enter PhD programmes in mathematics, computer science, or the applied sciences. Two streams run within the MSc, depending on whether a student wishes to focus on mathematics or on computation. The programme develops many skills valued by industry and it is possible to complete an MSc dissertation with an industrial partner.

A number of bursaries are available for highly qualified students.

The course starts in September and lasts one year. It comprises lectures and coursework, with exams in January and June, followed by a dissertation that is submitted in September. The dissertation counts for one half of the credits and is chosen from a range of available projects, including projects suggested by industrial partners.

Further information is available at

<http://www.maths.manchester.ac.uk/postgraduate/pgadmission/msc-mcs.html>

Enquiries should be addressed to: Programme Director Tony Shardlow (shardlow@maths.man.ac.uk)

Admissions Officer: Len Freeman (len.freeman@manchester.ac.uk)

University of Oxford

Oxford University Computing Laboratory and the Mathematical Institute offer a one-year full time M.Sc. course in Mathematical Modelling and Scientific Computing. This course aims to provide training in the applications of mathematics to a wide range of problems in science and technology. It is intended for graduates in mathematics or related disciplines wishing to pursue a career in industrial or commercial research or in academia.

The course consists of both taught courses and a dissertation. Topics covered include analytical and numerical solution of ordinary and partial differential equations, numerical linear algebra, numerical optimisation, mathematical ecology and biology, fluid dynamics and mathematical physiology,

The course is supported by EPSRC with 10-12 studentships being available each year.

We also offer a DPhil in Computer Science or Numerical Analysis.

For further details see <http://www.comlab.ox.ac.uk/oucl/courses/grad/mmsc>

University of Reading

The Department of Mathematics at the University of Reading offers two one-year taught postgraduate training courses, commencing on 1st October: **Mathematics of Scientific and Industrial Computation** (formerly Numerical Solution of Differential Equations) is running as a new course in the

Department of Mathematics. and **Mathematical and Numerical Modelling of the Atmosphere and Oceans**, run jointly with the Meteorology Department, which is fully funded by the NERC.

Applications are invited from candidates holding, or expecting to obtain, a minimum of a lower second class honours degree in mathematics or joint degree with mathematics, physics or engineering (with a significant mathematical content). Most qualified UK students would be eligible to receive funding of fees and stipend from the relevant research council, and most qualified EU students would be eligible for funding of fees.

Both courses are available on a part-time basis over two years.

For further details see <http://www.maths.rdg.ac.uk/> or contact Sue Davis, Postgraduate Secretary, Department of Mathematics, The University of Reading, Whiteknights PO Box 220, Reading RG6 6AX, UK. Tel: 0118 378 8991, email: S.Davis@rdg.ac.uk

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