

**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 Introduction

Welcome to spring edition of the IMA NA Newsletter. In this issue there is a chance to find out about the range of activities and research being carried out by the numerical analysts at the University of Reading. There is also an update on the HPC-NA Roadmap and an introduction to the Centre for Numerical Algorithms and Intelligent Software (NAIS).

The copy date for the next Newsletter will be **Friday 25 September**. Please do contribute! It would be great to have some short reports on some of the many interesting workshops and meetings that are taking place in the coming months (see the section on Highlighted Conferences and Workshops for details of some of these).

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2 Meet the Numerical Analysis Group ... Reading

Traditional activities in the Group have been computational fluid dynamics, numerical analysis of differential and integral equations and data assimilation and inverse problems. The relatively recent arrivals of Likhtman, Matsen, Grindrod and Tindall have led to a significant increase in computational modelling activities, in the areas of polymer physics and mathematical biology in particular. In addition to our research activities, we also run two MSc courses, “Mathematics of Scientific and Industrial Computation” and “Mathematical Modelling of the Atmosphere and Oceans”, the latter in collaboration with the meteorology department, each of which contains significant numerical analysis and computational modelling content. Members of the Group include:

Mike Baines, who continues to work on moving meshes, collaborating with Peter Jimack and Matthew Hubbard at the University of Leeds, and supervising PhD students Tamsin Lee (co-supervised by Stephen Langdon) and Anna Bebington (co-supervised by Paul Glaister) in Reading. The main thrust of the research is into finite element velocity-based methods for multidimensional time-dependent nonlinear PDEs and systems. Recent theoretical results concern preservation of scaling symmetry and the prediction of waiting times for nonlinear diffusion, whilst applications have included two-phase flows, avascular tumours and glacier models. The work is currently being written up for SIAM Review.

Timo Betcke has just started as an EPSRC funded postdoc in the Department of Mathematics, working with Simon Chandler-Wilde and Stephen Langdon on the numerical solution of high-frequency scattering problems. From 2002 to 2005 Timo Betcke was a DPhil student at the University of Oxford. He then worked as postdoc at the TU Braunschweig in Germany and The University of Manchester before coming to Reading in March 2009. His research interests include the numerical analysis of wave problems, eigenvalue computations and numerical linear algebra.

Simon Chandler-Wilde, whose research interests have a significant emphasis on the development and analysis of numerical algorithms for direct and inverse wave propagation problems. Currently this work focuses particularly on developing and analysing the use of novel basis functions for boundary and finite element methods that are adapted to high frequency problems where the solution is highly oscillatory. Another current emphasis is on developing methods for numerical solution of problems of rough surface scattering. Arising out of this second application, he has also recently been developing boundary integral equation method-based algorithms for free surface problems, and has been developing methods for computing the spectra of general bounded linear operators. This work has been funded in the last couple of years by EPSRC, NERC, the Leverhulme Trust, and the EU.

Sarah Dance is an RCUK Fellow in the Mathematics of Data Assimilation. Data assimilation refers to environmental state or parameter estimation, combining observations with numerical models. For example, data assimilation is used to provide initial conditions for numerical weather prediction models. Her particular interests lie in developing better data assimilation algorithms for storm and flood prediction, where the phenomena have highly nonlinear, multiscale characteristics, and the observations are heterogeneous in type and spatiotemporal frequency.

Peter Grindrod, whose research activities include the simulation of stochastic dynamics: analysis and

numerical simulation of cell motility using Othmer and Alt's "velocity jump" process models; and applying agent based simulation models to represent large customer base purchasing behaviour. In both cases it is the calibration problem at the microscopic scale conditioning on limited observations of macroscale behaviour that is challenging. Also, the analysis of dynamical networks: spectral theory of very large interaction matrices applied to problems of supervised clustering and the representation of observed datasets within certain classes of networks.

Steve Langdon has worked extensively in recent years on the design and analysis of methods for the numerical solution of high frequency scattering problems (in collaboration with Chandler-Wilde, as described above). Other recent work, in collaboration with Needham (Birmingham), has focused on the design and implementation of efficient schemes for computing the pressure and flow fields for a weakly compressible fluid flowing in a thin three-dimensional porous layer. Via a combination of matched asymptotic expansions and finite element methods, the full pressure and flow fields can be computed throughout the layer in a matter of minutes, compared to typical run times measured in hours for conventional solvers.

Amos Lawless is a research fellow of the NERC-funded National Centre for Earth Observation. His research interests lie in the numerical analysis of data assimilation algorithms for state estimation problems. In particular, he is concerned with developing new mathematical approaches to data assimilation for the very large, multi-scale problems which appear in environmental applications.

Alexei Likhtman and Mark Matsen lead the group of Theoretical Polymer Physics, which is concerned with theoretical and computational modeling of static and dynamic properties of polymer melts, block copolymers and other classical systems. They use a wide variety of numerical methods, including stochastic differential equations and molecular dynamics, as well as numerical solutions of partial differential equations in two and three dimensions.

Beatrice Pelloni has tutored masters students in various projects with computations of nonlinear waves using spectral methods. A recent highlight was work with Malachy McConnell on spectral computations of the solution to two dimensional integrable models of water waves (The DS equations). Apart from that, she is involved in a general plan for developing numerical schemes based on contour representations of the solution of evolution equations in one dimension.

Roland Potthast undertakes research on analysis and numerics for inverse problems. Inverse problems arise in a large variety of problems. The mathematics of inverse problems has developed into a broad and rich field, with various techniques for studying uniqueness and stability of reconstructions. Over the last years the inverse problems group has been one of the key players in developing novel algorithms for inverse problems, which have been applied to inverse scattering, electrical impedance tomography, magnetic tomography and inverse fluid dynamics. In particular, highly efficient sampling and probe methods have been developed both in the frequency and time domain to reconstruct unknown shapes and the structure of scattering objects. We are strongly involved in solving inverse problems in cognitive neuroscience. Here, a mesoscopic approach to brain dynamics is based on neural field theories, which model a large number of underlying neurons and their activity. Here, the group studies hierarchies of neural field equations and geometric effects which arise from incorporating local physiological effects like competition of neighboring neurons into brain dynamics.

Pete Sweby, who works on numerical schemes for conservation laws, at present with application to traffic flow, and currently supervises Bonhi Bhattacharya's work on Mathematical Modelling of Lipoprotein Metabolism.

Marcus Tindall works in the field of Mathematical Biology, developing mathematical models of biological and biomedical problems ranging from the single cell to whole organ scale in the fields of tumour growth, bacterial chemotaxis and lipoprotein (fat) metabolism. The models are deterministic and continuum in nature and more often than not with biological systems, highly non-linear. As a result we utilise a range of numerical code both readily available through packages such as Matlab and COMSOL (finite element), as well as implementing solvers for hyperbolic conservation laws. Recent examples include using the Weighted Average Flux method to solve problems in modelling in vitro tumours, utilising the COMSOL package to elucidate the role of diffusion and reaction kinetics in a bacterial signal transduction pathway and CLAWPACK to solve a system of hyperbolic equations in modelling the particles formed when fat is digested by the liver. In collaboration with colleagues from Oxford, Dr Tindall has also worked on hybrid cellular automata models for multi-scale problems. Individual cells are modelled using

cellular automata, each cell containing a system of ODEs describing the internal cell dynamics. This is then coupled to a PDE model describing extracellular factors such as the local nutrient supply. Such models can carry a high computational cost in terms of producing solutions in a feasible amount of time. A recent PhD student has investigated a number of approaches, including model reduction and discrete to continuum model comparisons, to overcome this.

3 HPC-NA Roadmap update

The third and final roadmap workshop was held at the Royal Society in London over 26th and 27th January 2009. There were 34 attendees, including four international participants. The initial draft version of the roadmap was presented and discussed at this workshop. A copy (together with reports on the each of the workshops) may be downloaded from <http://www.oerc.ox.ac.uk/research/hpc-na> This document is the outcome of the two community meetings in Oxford (November 2008) and Manchester (December 2008), together with input from similar activities elsewhere. The roadmap activity aims to provide a number of recommendations that together will drive the agenda toward the provision of:

- Algorithms and software that application developers can reuse in the form of high-quality, high performance, sustained software components, libraries and modules
- a community environment that allows the sharing of software, communication of interdisciplinary knowledge, and the development of appropriate skills.

The first version of the roadmap is built around five themes that have evolved during the discussions within the community.

- Theme 1: Cultural Issues
- Theme 2: Applications and Algorithms
- Theme 3: Software Engineering
- Theme 4: Sustainability
- Theme 5: Knowledge Base

As the roadmap activity goes forward, it is expected that these initial actions will develop into a detailed map of priorities across a sensible timeframe.

Comments and feedback on the roadmap are welcome and should be addressed to mark.hylton@oerc.ox.ac.uk

4 NAIS: Centre for Numerical Algorithms and Intelligent Software

At the end of 2008, EPSRC together with the Scottish Funding Council agreed to provide funds to establish the NAIS research centre as a joint venture of the University of Edinburgh, Heriot-Watt University and the University of Strathclyde. The total budget of NAIS is 8M GBP and the duration of the grant is 5 years, with first spending from August 2009.

What is the purpose of NAIS?

NAIS will bridge the gap between numerical analysts, computer scientists and HPC software developers by developing new systems of code annotation, new compilers and efficient implementations for application-oriented computational methods such as adaptive finite elements, multiscale modelling, molecular simulation and optimization.

Who is involved in NAIS?

NAIS is a partnership of the Schools of Mathematics and Informatics and the Edinburgh Parallel Computing Centre (EPCC) at the University of Edinburgh, and the Departments of Mathematics at Heriot-Watt and Strathclyde Universities. In addition, NAIS will include collaborations with researchers

in the sciences and engineering at the three universities, and a network of collaborations with other institutions including, so far, the University of Cambridge, the University of Warwick, and Wales Institute for Mathematics and Computer Science. A programme with CERFACS in Toulouse will provide for joint workshop and training activities. Industrial collaborations are to be established with IBM, Schlumberger, D.E. Shaw, SGI, Cray, Orage/France Telecom, SAS. An international advisory committee will be established.

The first director of NAIS is Benedict Leimkuhler (Mathematics, University of Edinburgh) and the Steering Committee consists of Mark Ainsworth (Mathematics, Strathclyde University), Murray Cole (Informatics, University of Edinburgh), Dugald Duncan (Mathematics, Heriot-Watt University), and Arthur Trew (Edinburgh Parallel Computing Centre).

What research activities are envisaged in NAIS?

NAIS will operate substantial training, visitor and workshop programmes in all relevant areas of numerical analysis, computer science and HPC software development. There will be additional activities at the NAIS partners.

What posts are anticipated in NAIS?

- 6 lectureships (permanent positions) in Mathematics (two each) at Edinburgh, Heriot-Watt and Strathclyde Universities.
- A lectureship in Informatics at the University of Edinburgh.
- 10 Postdoctoral Research Assistantships (3 years each).
- 24 PhD studentships (most 3 or 3.5, some 4 years duration).

The first posts will be advertised in Spring 2009. PhD student applications are welcome at any time and should be sent to the relevant department with a cover letter that mentions the “Numerical Algorithms and Intelligent Software Science and Innovation Project.

Where can I find out more about NAIS?

See <http://www.nais.org.uk/about> for further details. Specific queries may be sent to info@nais.org.uk.

5 Who's Visiting Whom

Bath

Ludmil Zikatanov (Penn State) will be visiting Bath in May.

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”.

Prof Nick Trefethen is hosting the following visits:

- Prof Roy Mathias (Birmingham), 19 January - 19 June 2009.
- Prof Gil Strang (MIT), 5 June - 4 July 2009.
- Prof Michael Overton (NYU), 13 July - 23 July 2009.

6 Technical Reports

University of Bath

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

- 03/09 A new multiscale Finite Element method for high-contrast elliptic interface problems.
C.-C. Chu, I. G. Graham and T.-Y. Hou.
- 02/09 Bayesian latent variable modelling in studies of air pollution and health.
Duncan Lee, Gavin Shaddick, Ruth Salway and Stephen Walker.
- 01/09 Scaling Up through Domain Decomposition.
C. Pechstein and R. Scheichl.
- 20/08 A model of shape memory alloys accounting for plasticity.
Martin Kruk and Johannes Zimmer.
- 19/08 A note on time-dependent DiPerna-Majda measures.
Martin Kruk and Johannes Zimmer.
- 18/08 Calculation of long time classical trajectories: algorithmic treatment and applications
for molecular systems.
Hartmut Schwetlick and Johannes Zimmer.

University of Cambridge

Reports available from http://www.damtp.cam.ac.uk/user/na/NA_papers.html

University of Edinburgh

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

- ERGO 09-001 K. Woodsend and J. Gondzio.
Hybrid MPI/OpenMP parallel support vector machine training.
- ERGO 09-002 X. Yang, J. Gondzio and A. Grothey.
Asset-liability management modelling with risk control by stochastic dominance.

University of Liverpool

Reports available from http://www.liv.ac.uk/~cmchenke/na_liverpool.htm

- 09/04 An Efficient Method for Evaluating the Integral of a class of highly oscillatory functions.
Paul J. Harris and Ke Chen.
- 09/05 A New Study of the Burton and Miller method for the Solution of a Three-Dimensional
Helmholtz Problem. Ke Chen, Jin Cheng and Paul J. Harris.

University of Manchester

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

- 2009.22: Françoise Tisseur, Seamus D. Garvey and Christopher Munro (2009).
Deflating Quadratic Matrix Polynomials with Structure Preserving Transformations.
- 2009.21: Nicholas J. Higham and Lijing Lin (2009).

On p th Roots of Stochastic Matrices.

- 2009.15: Younes Chahlaoui (2009).
Model reduction of switched dynamical systems. In: 4th Conference on Trends in Applied Mathematics in Tunisia, Algeria and Morocco, 6-8 May 2009, Kenitra, Morocco.
- 2009.14: Younes Chahlaoui (2009).
A new approach for MOR of second order Dynamical Systems. In: Systems Theory: Modelling, Analysis and Control, 25-28 May 2009, Fes, Morocco.
- 2009.12: Younes Chahlaoui (2009).
A posteriori error bounds for discrete balanced truncation. SIAM Journal on Scientific Computing (SISC).
- 2009.11: David R Stephenson, John L Davidson, William R.B. Lionheart, Bruce D Grieve and Trevor A York (2005).
Comparison of 3D Image Reconstruction Techniques using Real Electrical Impedance Measurement Data. Proceedings of the 4th World Congress on Industrial Process Tomography. pp. 643-650.
- 2009.9: Awad H. Al-Mohy and Nicholas J. Higham (2009).
A New Scaling and Squaring Algorithm for the Matrix Exponential.
- 2009.8: Yinan Li, Jack Dongarra and Stanimire Tomov (2009).
A Note on Auto-tuning GEMM for GPUs.
- 2009.7: Stanimire Tomov, Jack Dongarra and Marc Baboulin (2009).
Towards Dense Linear Algebra for Hybrid GPU Accelerated Manycore Systems.
- 2009.6: Hatem Ltaief, Jakub Kurzak and Jack Dongarra (2009).
Parallel Block Hessenberg Reduction using Algorithms-By-Tiles for Multicore Architectures Revisited.
- 2009.5: Hatem Ltaief, Jakub Kurzak and Jack Dongarra (2009).
Parallel Band Two-Sided Matrix Bidiagonalization for Multicore Architectures.
- 2009.4: Jack Dongarra and Julien Langou (2009).
The Problem with the Linpack Benchmark 1.0 Matrix Generator.
- 2009.3: George Bosilca, Remi Delmas, Jack Dongarra and Julien Langou (2009).
Algorithmic Based Fault Tolerance Applied to High Performance Computing.
- 2009.2: Marc Baboulin, Jack Dongarra and Stanimire Tomov (2009).
Some Issues in Dense Linear Algebra for Multicore and Special Purpose Architectures.
- 2009.1: Gareth I. Hargreaves (2002). Interval Analysis in Matlab.

University of Oxford

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

- NA-09/01 On solving trust-region and other regularised subproblems in optimization.
H. Sue Dollar, Nicholas I. M. Gould, and Daniel P. Robinson.

Rutherford Appleton Laboratory

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

- RAL-TR-2009-007 J. A. Scott. A note on a simple constrained ordering for saddle-point systems.
- RAL-TR-2009-006 C. Cartis, N. I. M. Gould and Ph. L. Toint.
An adaptive cubic regularization algorithm for nonconvex optimization with convex constraints and its function-evaluation complexity.
- RAL-TR-2009-004 J. D. Hogg, J. K. Reid and J. A. Scott.
A DAG-based sparse Cholesky solver for multicore architectures.
- RAL-TR-2009-003 H. S. Dollar, N. I. M. Gould and D. P. Robinson. On solving trust-region and other regularised subproblems in optimization.
- RAL-TR-2009-002 N. I. M. Gould and D. P. Robinson.
A second derivative SQP method: local convergence.
- RAL-TR-2009-001 N. I. M. Gould and D. P. Robinson.
A second derivative SQP method: global convergence.

7 Diary of Seminars (April 2009 - July 2009)

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/mathsevents>

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://talks.cam.ac.uk/show/index/9811>), 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://talks.cam.ac.uk/show/index/15177>).

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>

LIVERPOOL : Seminars are normally held on Wednesdays at 4pm, in the Whittaker Room (211), Mathematical Sciences Building.
See <http://www.liv.ac.uk/math/Applied/Research/Seminars/index.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: sue.dollar@stfc.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.

Please note that, at the time of writing, not many people had fully sorted out their seminar series for this coming term so you are advised to check the given websites for details of titles and of further seminars as they become available.

APRIL 2009

April 23 : RAL. Coralia Cartis (Edinburgh).

April 24 : BATH. Emily Dodgson (Bath).

April 24 : MANCHESTER. Christian Mehl (Birmingham).

April 24 : READING. Moss Mokgolele (Reading). Numerical Solution of High Frequency Acoustic Scattering Problems

April 29 : LIVERPOOL. B J Matuszewski (Central Lancashire). Biomedical Computer Vision.

April 29 : EDINBURGH. Joanne Carr (Daresbury Laboratory).

April 30 : OXFORD. Andrew Stuart (Warwick).

MAY 2009

May 1 : BATH. Chris Hart (Bath).

May 1 : READING. Jenya Ferapontov (Loughborough). Soliton equations in 2+1 dimensions: deformation of dispersionless limits.

May 7 : OXFORD. John Appleyard (Polyhedron).

May 8 : BATH. Nicolette Rattenbury (Manchester Metropolitan).

May 8 : EDINBURGH. Karsten Neuhoff (Cambridge).

May 14 : OXFORD. Ivan Graham (Bath).

May 15 : BATH. Ludmil Zikatanov (Pennsylvania State).

May 15 : READING. Larissa Fradkin (London South Bank). Semi-analytical modelling of diffraction by surface-breaking cracks, with application to ultrasonic inspection of nuclear power plants.

May 22 : READING. Eric Darrigrand (Rennes).

May 29 : READING. Mahadevan Ganesh (Colorado School of Mines). Simulation of electromagnetic interactions with multiple three dimensional particles.

JUNE 2009

June 1 : BRUNEL. Rob Douglas (Aberystwyth). Applications of Optimal Mass Transportation to Geophysics.

June 4 : RAL. Amos Lawless (Reading).

June 5 : BATH. Kerstin Hesse (Sussex).

June 15 : BRUNEL. Victor Shrira (Keele).

8 Forthcoming Meetings and Conferences

MAY 2009

4th International Conference on Grid and Pervasive Computing (GPC 2009), May 4-8.

Geneva, Switzerland. <http://gpc09.eig.ch/>

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 Engineering and Computational Mathematics (ECM2009), May 27-29.

The Hong Kong Polytechnic University. <http://www.polyu.edu.hk/ama/events/conference/ECM2009/>

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

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

JUNE 2009

CTW09 - 8th Cologne-Twente Workshop on Graphs and Combinatorial Optimization, June 5-5.

Paris. <http://www.lix.polytechnique.fr/ctw09/>

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

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

BICS workshop: Reflections in Nonlinear Mechanics, June 8-9.

University of Bath. <http://www.bath.ac.uk/math-sci/bics/conferences/index.html>

The 2nd International Conference on Mathematical Modelling and Computation and The 5th East Asia SIAM Conference, June 8-11.

Universiti Brunei Darussalam (UBD) <http://mmc09.ubd.edu.bn/>

23rd International Conference on Supercomputing, June 9-11.

IBM T.J. Watson Research Center Metro New York City Area, USA. <http://www.ics-conference.org>

MAFELAP 2009, the Thirteenth Conference on the Mathematics of Finite Elements and Applications, June 9-12.

Brunel University. <http://people.brunel.ac.uk/icsrssi/bicom/mafelap2009>

Conference on Scientific Computing and Differential Equations celebrating Ernst Hairer's 60th birthday, June 17-19.

University of Geneva, Switzerland. <http://www.unige.ch/math/hairer60/>

Mathematical Modelling and Computational Methods in Applied Sciences and Engineering, June 22-26.

Roznov pod Radhostem, Czech Republic <http://www.ugn.cas.cz/link/modelling09>

8th International Conference on Spectral and High Order Methods (ICOSAHOM), June 22-26.

Trondheim, Norway. <http://www.math.ntnu.no/icosahom>

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

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

Reliable Methods of Mathematical Modeling, June 24-26.

Berlin, Germany <http://www.math.hu-berlin.de/~rmmm2009>

European Conference on Numerical Mathematics and Advanced Applications, (ENUMATH 2009) June 29 - July 3.

Uppsala, Sweden. <http://www.akademikonferens.uu.se/enumath2009/>

14th Leslie Fox Prize meeting, June 29.

University of Warwick. <http://www.warwick.ac.uk/~masdr/fox/>

9th Conference on Computational and Mathematical Methods in Science and Engineering June 30 - July 3.

Gijon, Asturias, Spain. <http://xixon.epv.uniovi.es/cmmse09/>

BICS workshop: Multiply Structured Biological Systems, July 1-3.

University of Bath. <http://www.bath.ac.uk/math-sci/bics/conferences/index.html>

JULY 2009**EURO XXIII- 23rd EURO Conference on Operations Research, July 5-8.** Bonn, Germany.

<http://www.euro-2009.de/>

SIAM Conference on Control and Its Applications (CT09), July 6-8. Denver, Colorado.

<http://www.siam.org/meetings/ct09/>

SIAM Annual Meeting (AN09), July 6-10. Denver, Colorado.

<http://www.siam.org/meetings/an09/>

Workshop on Matrix Analysis and Applications, July 9-13. Zhejiang Forestry University, Hangzhou, China. <http://www.nova.edu/>**Sparse Matrices for Scientific Computation: In Honour of John Reid's 70th Birthday, July 15-16.**

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

8th European Automatic Differentiation Workshop, July 17.

The Numerical Algorithms Group, Oxford. <http://www.autodiff.org/euroad/8>

BICS workshop: Animal Social Networks, July 20-22.

University of Bath. <http://www.bath.ac.uk/math-sci/bics/conferences/index.html>

AUGUST 2009**Modeling and Optimization: Theory and Applications (MOPTA 2009), August 19-21.** Lehigh University, Bethlehem, PA.**20th International Symposium of Mathematical Programming (ISMP), August 23-29.** Chicago, Illinois. <http://www.ismp2009.org/>**Preconditioning 2009, August 24-26.**

Hong Kong. <http://www.math.hkbu.edu.hk/precond09/index.html>

EURO-PAR 2009, August 25-28.

Delft University of Technology, The Netherlands. <http://europar2009.ewi.tudelft.nl/>

Algorithms for Approximation VI, August 31- September 4.

Ambleside, Lake District, UK.

<http://www2.le.ac.uk/departments/mathematics/extranet/conferences>

SEPTEMBER 2009**Euro PVM/MPI 2009 meeting, September 7-10.**

Espoo, Finland. <http://www.csc.fi/english/pages/pvmmpi09/welcome>

38th SPEEDUP Workshop on High Performance Computing, September 7-8.

EPF Lausanne, Switzerland. <http://www.speedup.ch/>.

9th GAMM Workshop on Applied and Numerical Linear Algebra, September 10-11.

ETH Zurich, Switzerland. <http://www.sam.math.ethz.ch/GAMM09/>

12th Seminar NUMDIFF on Numerical Solution of Differential and Differential-Algebraic Equations, September 14-18.

CWI, Amsterdam. <http://www.mathematik.uni-halle.de/numdiff>

6th Conference on Applied Mathematics and Scientific Computing, September 14-18.

Zadar, Croatia <http://www.math.hr/~rogina/ApplMath09/first.html>

14th Belgian-French-German Conference on Optimization (BFG09), September 14-18.

Leuven, Belgium. <http://www.kuleuven.be/bfg09>

BICS workshop: The Future of Complexity Science, September 15-16.

University of Bath. <http://www.bath.ac.uk/math-sci/bics/conferences/index.html>

Inter. Conf. on Optimization and Applications (OPTIMA2009) , September 21-25. Petrovac,

Montenegro. <http://www.ccas.ru/optima2009>

22nd Chemnitz FEM Symposium, September 28-30. Chemnitz, Germany.

<http://www.tu-chemnitz.de/mathematik/fem-symposium/>

OCTOBER 2009**SIAM Conference on Mathematics for Industry: Challenges and Frontiers (MI09),**

October 5-8. San Francisco, USA. <http://www.siam.org/meetings/mi09/>

Woudschoten Numerical Analysis Conference, October 7-9.

Woudschoten Conference Centre, Zeist, The Netherlands.

<http://wsc.project.cwi.nl/conferentieE.php>

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

Seaside, California. <http://www.siam.org/meetings/la09>

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

Seaside, California. <http://www.siam.org/meetings/cs09>

DECEMBER 2009**SIAM Conference on Analysis of Partial Differential Equations (PD09),**

December 7-9. Miami, Florida. <http://www.siam.org/meetings/pd09/>

9 Highlighted Conferences and Workshops

MAFELAP 2009: June 9th - 12th 2009 Brunel University, UK

We are pleased to announce that MAFELAP 2009, the Thirteenth Conference on the Mathematics of Finite Elements and Applications, will take place at Brunel University during the period 9 - 12 June, 2009. This conference is dedicated to Mary Wheeler and John Whiteman, both having reached the age of 70. The aim is to bring together workers from different disciplines whose common interest is finite element methods, and to promote wider awareness throughout the finite element community of the latest developments in the field.

The invited speakers will include:

- J Barrett, Imperial College, London.
- S Chandler-Wilde, Reading University
- P Jimack, University of Leeds
- S Mikhailov, Brunel University
- K Morgan, Swansea University
- JT Oden, University of Texas at Austin
- O Pironneau, University of Paris VI (Pierre et Marie Curie)
- E Suli, Oxford University
- A Tessler, NASA, Langley Research Center.

Whilst many have already been proposed, we are still encouraging colleagues to propose Mini-Symposia which they would like to organise at MAFELAP. Briefly, the parameters for a mini-symposium are that we shall allocate a time-slot to the organisers, during which they can have four speakers, each giving a presentation (probably 30 minutes, 25 minutes talk plus 5 minutes for questions). If organisers want more than four talks, then we could give them two two-hour slots. If you are interested in running a mini-symposium, please submit a title as soon as possible, with a tentative list of speakers to Professor Norbert Heuer (nheuer@mat.puc.cl) or Carolyn Sellers (carolyn.sellers@brunel.ac.uk).

Full details of the conference together with registration forms can be found at:
<http://people.brunel.ac.uk/~icsrsss/bicom/mafelap2009>

MAFELAP 2009 Studentships

As a result of a grant from the Institute of Mathematics and Its Applications (IMA) the conference is able to fund a number of MAFELAP 2009 Studentships for research students who are studying at universities in the UK and the Republic of Ireland, who do not have other means of support. These studentships will cover the registration fees at the conference (not accommodation or travel). Applications are now invited, and any student wishing to apply for a studentship should, not later than 1 May 2009, submit a Case for Support (not more than 1 A4 page) together with a supporting letter from his/her supervisor to mafelap2009@brunel.ac.uk.

Carolyn Sellers
MAFELAP Secretary
Brunel University, UK
mafelap2009@brunel.ac.uk

**23rd Biennial Conference on Numerical Analysis
June 23rd - 26th 2009
University of Strathclyde**

The following distinguished researchers have accepted invitations to deliver plenary lectures at the conference.

- Annalisa Buffa (IMATI-CNR Pavia)
- Gerd Dziuk (Freiburg University)
- Ernst Hairer (Universite de Geneve)
- Matthias Heinkenschloss (Rice University)
- Ralf Hiptmair (ETH Zurich)
- Ilse Ipsen (North Carolina State University)
- Peter Jimack (University of Leeds)
- Karl Kunisch (University of Graz)
- Ulrich Langer (University of Linz)
- Jesus Maria Sanz-Serna (University of Valladolid)
- Larry Schumaker (Vanderbilt University)
- Charles Van Loan (Cornell University)

The A R Mitchell lecture will be given by Larry Schumaker.

The after dinner speaker will be Alistair Watson (University of Dundee).

For full details, see <http://www.maths.strath.ac.uk/naconf/>

**Numerical and analytical solution of stochastic delay differential equations
7th 11th September 2009
Department of Mathematics, University of Chester**

The Leverhulme International Network based at the University of Chester presents a research meeting on stochastic delay differential equations in Chester in September 2009. Full details will be available shortly. Please contact us to be added to the mailing list and for further details.

The Leverhulme International Network, based in Chester and led by Professor Neville Ford, has been established for 3 years from 2008 to 2011, with the aim of bringing together experts from the areas of mathematical modelling, mathematical analysis, numerical and computational methods and stochastic analysis of functional differential equations. This is the 2nd of 4 network workshop meetings to enable methodologies to be shared and new working methods and collaborations to be established.

Scientific queries to: Neville Ford (njford@chester.ac.uk).

Other queries should be addressed to Nicola Williams (nicola.williams@chester.ac.uk).

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

This meeting will bring together leading numerical analysts from the UK and abroad in honour of John Reid's 70th birthday. John is an eminent UK numerical analyst who, over a career spanning five decades, has made many important contributions, particularly in the development of sparse matrix technology. His main contributions include: conjugate gradients as an iterative method, Markowitz' pivoting for sparse matrices, estimating sparse Jacobians, factorizing and updating linear programming bases, steepest-edge simplex algorithm, the multifrontal method for sparse linear systems, using 2×2 pivots for sparse symmetric indefinite matrices, and ordering sparse matrices for small wavefront and profile.

The speakers will be:

- Andrew Cliffe, University of Nottingham.
- Jack Dongarra, University of Tennessee. *PLASMA and Scheduling Dense Linear Algebra on Multicore Chips.*
- Iain Duff, FRSE, STFC Rutherford Appleton Laboratory
- Al Erisman, Seattle Pacific University.
- Roger Fletcher, FRS FRSE, University of Dundee. *L-Implicit-U factorization and the Simplex Update.*
- Shaun Forth, Cranfield University. *Automatic Differentiation and Sparse Matrices.*
- Ian Gladwell, Southern Methodist University, Dallas. *ACM Transactions on Mathematical Software Past, Present and Future.*
- Sven Hammarling, Principal Consultant at NAG
- Kaj Madsen, Technical University of Denmark.
- Nancy Nichols, University of Reading.
- Beresford Parlett, University of California.
- Michael Powell, FRS, University of Cambridge. *How many function values are sufficient to estimate the least value of a quadratic function.*
- John Reid, STFC Rutherford Appleton Laboratory.
- Michael Saunders, Hon FRSNZ, Stanford University. *Some sparse LU considerations.*
- Jennifer Scott, STFC Rutherford Appleton Laboratory. *Too large to handle directly?*
- Nick Trefethen, FRS, Oxford University. *Spectral accuracy and conformal maps.*

The meeting will be held at Cosener's House. Cosener's House occupies a picturesque Thames side position in the grounds of the ancient abbey of Abingdon in south Oxfordshire. Please note that the number of places available at this meeting is limited so early registration is advised. Thanks to partial funding from the IMA and the LMS, we are able to offer a special rate for students and postdocs.

Closing date for registration: **1 June.**

For further details and to register, please go to <http://www.numerical.rl.ac.uk/people/hsd/jkr/>

8th European AD Workshop

Delegates of the Sparse Matrices for Scientific Computation Conference may also be interested in attending the 8th European AD Workshop in Oxford on 17 July 2009. This 1-day workshop continues the series of EuroAD Automatic Differentiation workshops, taking place twice a year. EuroAD workshops are organized jointly by the University of Hertfordshire, Cranfield University in Shrivenham, RWTH Aachen University (Germany), and INRIA Sophia-Antipolis (France).

The workshop is kindly being hosted by the Numerical Algorithms Group (NAG) in Oxford, UK. For further details see URL: <http://www.autodiff.org/euroad/8>

10 Software News

HPC training for UK researchers

The HECToR Service is pleased to announce more free High Performance Computing (HPC) training at locations around the UK.

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 Fortran 95, 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 and locations please see:
<http://www.hector.ac.uk/cse/training/>

A full list of available courses and contact details are here:
<http://www.hector.ac.uk/cse/training/courselist/>

For more information about HECToR and the CSE service please see
<http://www.hector.ac.uk/> and <http://www.hector.ac.uk/cse/>

The HECToR CSE Team

Operations Research Group Edinburgh

The Operations Research Group at the University of Edinburgh has for many years implemented and produced several packages of computer software mostly for optimization problems. Our latest release is SML (Structured Modelling Language), an implementation of a structure-conveying extension to the AMPL modelling language (contact author: Andreas Grothey).

SML extends AMPL with object-oriented features that allow to construct models from sub-models. Unlike traditional modelling languages, the new approach does not scramble the block structure of the problem, and thus it enables the passing of this structure on to the solver. Its design allows the problem generation phase to be parallelisable.

Other computer software packages produced and available are:

HOPDM (Higher Order Primal-Dual Method) is Jacek Gondzio's implementation of an infeasible primal-dual path-following interior point method for linear, convex quadratic and convex nonlinear programming problems.

OOPS (Object-Oriented Parallel Solver) is a parallel interior point code that exploits any special structure in the Hessian and Jacobian matrices, developed by Jacek Gondzio, Andreas Grothey and Robert Sarkissian.

EMSOL is an implementation of the simplex method written and maintained by Julian Hall.

More information about each package can be found at <http://www.maths.ed.ac.uk/ERGO/software.html>

NAG

By the time I am asked to contribute another Software News from NAG article I shall be announcing the releases of new Fortran Libraries. Currently NAG is whetting appetites around the country by giving courses demonstrating and describing the new materials.

The latest of these was kindly hosted by the Business School in Manchester University. It featured three non-NAG speakers:

- Simon Acomb spoke on “Correlation in practice: products, estimation and importance of being positive semi-definite”
- Nicholas Higham talked about “Structured Nearest Correlation Matrix Problems” and
- Michael Croucher helped me explain how to get the most from NAG DLL libraries by also using them from Excel.

Simon and Nicholas were able to refer to the forthcoming nearest correlation routine G02AAF whilst a NAG speaker, Robert Tong, was able to speak about the derivative pricing routines becoming available in our S chapter at Mark 22.

Materials relating to the course, which also included exercises and solutions, are posted on the NAG web-site at: http://www.nag.co.uk/market/training/manchester_finance_feb09/

If you visit this link you will see that Craig Lucas from NAG also spoke about the NAG Toolbox for MATLAB. Of course, whenever we update the libraries, the toolbox is updated too. Our web site: http://www.nag.co.uk/NAGNews/NAGNews_Issue78.asp#Article4 points to updated complete MATLAB demonstrations of NAG routines. These have proved to be very popular downloads. We have additional demonstration material ready to be added just as soon as the new NAG Toolboxes become available.

The next free courses we have planned will be hosted at the NAG offices and will again centre around the MATLAB and Excel packages. Please look out for announcements about courses on 7th May and 10th June or, if you think you would be interested and want to be sure of a place, please contact Katie O’Hare at katie.o'hare@nag.co.uk

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

11 PhD Theses

Bath

Richard Norton. Numerical Computation of Band Gaps in Photonic Crystal Fibres.
(<http://www.maths.ox.ac.uk/ldapcontact/userdetails/norton>)

Zhivko Stoyanov. Spectral Graph Theory and Algorithms for Networks.
(<http://people.bath.ac.uk/mapzvs/>)

Liverpool

Noor Badshah. Fast Iterative Methods for Variational Models in Image Segmentation.

Oxford

Martin Stoll. Solving linear systems using the adjoint.

12 Recent Appointments

Euan Spence started working as a postdoc on 24 March 2009. He will be working on the project: Boundary Integral Equation Methods for High Frequency Scattering Problems. See <http://www.maths.bath.ac.uk/~igg/HF/>

13 Vacant positions and studentships

University of Liverpool: Teaching Assistantships

In partnership with the Xi'an Jiaotong-Liverpool University (XJTLU), the Department of Mathematical Sciences at the University of Liverpool has the fortunate and rare chance of having 4 vacancies of teaching assistantships (TAs). The successful candidates will register for a 4 year PhD programme within the remit of the department's research activities, including Numerical Analysis. For full details see http://www.liv.ac.uk/math/Prosp_PG/index.html The deadline for applications is 30 April 2009. General contact: Ms S Farell safrell@liverpool.ac.uk

PhD Studentships at Edinburgh, Heriot-Watt and Strathclyde Universities

A number of PhD studentships will be available either supported directly by NAIS or affiliated to NAIS (Centre for Numerical Algorithms and Intelligent Software). Several targeted projects are listed below. Students interested in PhD work on NAIS-relevant themes are encouraged to apply even if their interests do not directly connect with the projects listed. Applicants wishing to be considered for NAIS funding should mention that fact in their cover letter.

NAIS PhD Studentship: Multi-site Performance Optimisation for Parallel Programs For more information contact Murray Cole (mic@inf.ed.ac.uk).

NAIS PhD Studentship: Adaptive Parallel Optimising Compilation using Machine Learning. For more information contact Mike OBoyle (mob@inf.ed.ac.uk).

NAIS PhD Studentship: Domain Decomposition Preconditioners For more information contact Mark Ainsworth (m.ainsworth@strath.ac.uk).

NAIS-Affiliated PhD Studentship: The Application of Molecular Dynamics to Structural Chemistry Problems For more information contact Ben Leimkuhler (b.leimkuhler@ed.ac.uk).

Further information and details of other NAIS vacancies are available at <http://www.nais.org.uk/vacancies>

14 Postgraduate Courses

Please refer to the newsletters from October 2008 and January 2009 (available at http://www.ima.org.uk/learned_soc/interestgroups.htm) for details of postgraduate courses (including those that will commence in October 2009).

15 IMA Journal of Numerical Analysis

Contents of Volume 29, Number 1

- 1-23 Karl Deckers and Adhemar Bultheel.
Recurrence and asymptotics for orthonormal rational functions on an interval.
- 24-42 Bjrn Fredrik Nielsen, Aslak Tveito, and Wolfgang Hackbusch.
Preconditioning by inverting the Laplacian: an analysis of the eigenvalues.
- 43-71 Jeongho Ahn and David E. Stewart.
Dynamic frictionless contact in linear viscoelasticity.
- 72-85 Radu-Alexandru Todor.
A new approach to energy-based sparse finite-element spaces.
- 86-108 Gabriel N. Gatica, Salim Meddahi, and Ricardo Oyarza.
A conforming mixed finite-element method for the coupling of fluid flow with porous media flow.
- 109-125 Torsten Lin and Niall Madden.
Layer-adapted meshes for a linear system of coupled singularly perturbed reaction diffusion problems.
- 126-140 Ricardo H. Nochetto, Andreas Veerer, and Marco Verani.
A safeguarded dual weighted residual method.
- 141-157 A. Amiraslani, R. M. Corless, and P. Lancaster.
Linearization of matrix polynomials expressed in polynomial bases.
- 158-179 W. Hackbusch, W. Kress, and S. A. Sauter.
Sparse convolution quadrature for time domain boundary integral formulations of the wave equation.
- 180-207 Erwin Hernandez, Enrique Otrola, Rodolfo Rodriguez, and Frank Sanhueza.
Approximation of the vibration modes of a Timoshenko curved rod of arbitrary geometry.
- 208-234 Arie C. de Niet and Fred W. Wubs.
Numerically stable LDLT-factorization of F-type saddle point matrices.

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

16 Acknowledgements

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