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Numerical Analysis Reports

DEPARTMENTS OF MATHEMATICS

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Contents

This Annual Report serves to publicize the work that has taken place in the Manchester Centre for Computational Mathematics during 2003. *Along with other MCCM technical reports, information about the M.Sc. in Applied Numerical Computing, and MCCM seminar details, it is available from the MCCM Web page at* `http://www.ma.man.ac.uk/MCCM`

Edited by F. Tisseur

1 A Message from the Director

The main event of the year for MCCM was the workshop *New Frontiers in Computational Mathematics* held at Chancellors Hotel and Conference Centre at the University of Manchester in January 2004. (Since the workshop fell just a few days outside the year covered by this report, it seemed natural to include it here.) Generously sponsored by the University of Manchester, the London Mathematical Society, the UK and Republic of Ireland SIAM Section, the Royal Society and the Wolfson Foundation, the meeting brought 63 participants to Manchester for spirited discussion about computational mathematics and its many applications. Particularly notable was the interdiscplinary focus, with attendees from computer science, engineering, biological sciences, and medicine. A report on the conference can be found in Section 5.

Much work is underway on the merger between the Victoria University of Manchester and UMIST, which will create the new *University of Manchester* in October 2004. In the new School of Mathematics, the Numerical Analysis Group will contain eight members of staff, making it one of the largest and broadest numerical analysis Groups in the UK. Buoyant applications for postgraduate study in NA, together with continuing funding successes from the group members, bode well for the future of the subject in Manchester. Turning to the past, I feel it is important that the history of numerical analysis is not lost as time goes on and those who created and developed it retire. To this end, Joan Walsh kindly took up my invitation to write an article about the early history of NA at the University of Manchester. Joan, who recently retired, formed and for many years led the NA group at the University, and served also as Head of Department and Pro-Vice Chancellor. You will find Joan's interesting article in Section 4.

Nicholas J. Higham
Director of MCCM

2 Members

Christopher T. H. Baker

Professor of Mathematics, University of Manchester
D.Phil., Oxford University, 1964

I continue at Manchester University as Research Professor on a part-time salary; my links with University College Chester continue to thrive. In January, I reached the age of $64_{10} = 1000000_2$. (It is only a personal view, but as the smallest 7-digit binary number, I regard the decimal 64 as a candidate for a celebration at least as much as the multiples of 5 – at least, those between 60 and 95 – traditionally chosen as grounds for festivity!)

My collaborators have included Drs Evelyn Buckwar (Humboldt University), Judy Ford (UMIST & Chester), Chris Paul, Fathalla Rihan (Salford), and Yihong Song (Suzhou University Shanghai) and Professors Genna Bocharov (Moscow, Leverhulme Professor at University College Chester), Neville Ford (University College Chester), and Pat Lumb and Stewart Norton at Chester.

My interest in stochastic delay differential equations continued with work on bifurcation that in 2002 resulted in an MCCM Technical Report [396] and subsequently a paper now accepted for publication, due to appear in September 2004. During the year, I visited Dr Evelyn Buckwar in Berlin. I spoke at an analysis meeting held in the summer at Dublin City University; this enabled renewed contact with Dr John Appleby who works on stochastic delay differential equations. I also attended NUMDIFF 10 in Wittenberg, where I gave a talk on the work on model identification in which I have been engaged with Genna Bocharov, Chris Paul, and Fathalla Rihan.

I have continued links with Hagen Gilsing, a PhD student at the Humboldt University in Berlin, and continued the supervision in Manchester of Eugene (Evgeny) Parmuzin. The collaboration with my former PhD student Dr Yihong Song has resulted in six papers accepted for publication, two of which appeared this year (see below).

- The numerical solution of stochastic delay differential equations, with Dr Buckwar, and with Professor Neville Ford and Dr Judy Ford.
- Mathematical models with time-lag in the biosciences, with Prof Genna Bocharov, Dr Chris Paul and Dr Fathalla Rihan, Pat Lumb and Stewart Norton; parameter identification methodologies, sensitivity, etc.
- Identification of the initial function in modelling with DDEs (with Eugene Parmuzin). The reduction of an identification problem to an integral equation, and discrete analogues.
- The solution of discrete Volterra equations, with Dr Yihong Song, now in Shanghai.
- The numerical solution of neutral and delay differential equations, with Dr Paul: discontinuous solutions of NDDEs in Hale's form.

Appointments and Professional Activities

I am endeavouring to reduce the number of my commitments, but during the year I have been:

1. Research professor (part-time)
2. Professor emeritus, University of Manchester.
3. Visiting professor, Chester College
4. Founding-director, MCCM
5. Member of the College of the EPSRC Mathematic Programme
6. Editor, Journal of Computational & Applied Mathematics
7. Editor, Journal of Integral Equations & Applications
8. Member of the accreditation board, Computer Abstracts
9. Referee for a number of journals and publishers.

Publications

1. Baker, C. T. H. and Song, Y., Discrete Volterra Operators – Fixed Point Theorems & their Application, Nonlinear Studies, 10 (2003), 79-101.
2. Song, Y. and Baker, C. T. H., Perturbation Theory for Discrete Volterra Equations, Journal of Difference Equations and Applications, 9 (2003), pp. 969-987.

Numerical Analysis Reports

425 C. T. H. Baker, G. A. Bocharov, C. A. H. Paul and F. A. Rihan, Models with Delays for Cell Population Dynamics: Identification, Selection and Analysis – Part I, February 2003.

430 C T H Baker and E I Parmuzin A Guided Tour of Variation of Parameters Formulae for Continuous and Discretized DDEs, September 2003.

431 C T H Baker and E I Parmuzin Identification of the initial function for delay differential equations. Part I: The continuous problem and an integral equation analysis. September 2003

Lectures

1. Invited plenary talk, 5th Dublin Differential Equations Conference, Dublin City University: `http://www.deconf.dcu.ie/ddec_program.pdf`

2. Invited plenary talk, NUMDIFF10, Halle September 2003: `http://sim.mathematik.uni-halle.de/~numdiff/Numdiff10/`

Research Grants

Scheme 4 grant from London Mathematical Society.

Gennady A. Bocharov

Leverhulme International Visiting Professor, Mathematics Department, University College Chester
Ph.D. Department of Numerical Mathematics, USSR Academy of Sciences, 1985

I have continued collaborative research on applications of mathematics to immunology. I collaborated with John Edwards, Neville Ford, Pat Lamb, Stewart Norton (Mathematics Department) and John Williams (Biology Department) at Chester and, Christopher Baker and Chris Paul (University of Manchester). Other collaborative links involve Burkhard Ludewig (St. Gallen, Switzerland), Andreas Meyerhans (Homburg, Germany), Paul Klenerman (Oxford), Stephan Ehl (Freiburg, Germany). Some of my work was presented at St. Gallen Conference of the Swiss Society for Immunology in March 2003, at Ekaterinburg meeting on Mathematics and Immunology in May 2003, at Edinburgh Meeting on Computational Modelling in Medicine in September 2003, at Berlin Conference of the German Society for Immunology in September 2003 and at a seminar of the Biology Department of the Royal Holloway in December 2003.

Appointments and Professional Activities

Leading Researcher, Institute of Numerical Mathematics, Russian Academy of Sciences, Moscow.

Honorary Research Fellow, University of Manchester.

Honorary Research Fellow, Imperial College of Science, Technology and Medicine, London.

Publications

A. Meyerhans, A. Jung, R. Maier, J.P. Vartanian, G. Bocharov, S. Wain-Hobson. The non-clonal and transitory nature of HIV in vivo. *Swiss Med. Weekly.*, 133(33-34):451–454, 2003.

B. Ludewig, P. Krebs, T. Junt and G. Bocharov. Dendritic cell homeostasis in the regulation of self-reactivity. *Current Pharmaceutical Design*, 9:221–231, 2003.

G. Bocharov, P. Klenerman and S. Ehl. Modelling the dynamics of LCMV infection in mice: II. Compartmental structure and immunopathology. *Journal of Theoretical Biology*, 221:349–378, 2003.

G. Bocharov, B. Ludewig, A. Bertoletti, P. Klenerman, T. Junt, P. Krebs, T. Luzyanina, C. Fraser, and R.M. Anderson. Underwhelming the Immune Response: Effect of Slow Virus Growth on CD8+-T- Lymphocyte Responses. *Journal Virology*, 78:2247–2254, 2004.

Research Grants

I received a research grant from the Russian Foundation of Basic Research supporting collaborative research on *Numerical modeling of virus infection dynamics using functional differential equations*

Philip I. Davies

Research Associate, University of Manchester
Ph.D. University of Manchester, 2000

I have successfully completed the EPSRC-funded project "Numerical Analysis of Matrix Functions". A final report on the project is available to download on the project website `http://www.maths.man.ac.uk/~higham/NAMF`.

In 2003, I worked with Professor Nick Higham on the problem of computing $y = f(A)b$ for various matrix functions f. We investigated a general method that applies quadrature to the matrix version of the Cauchy integral theorem. Also, we investigated specific methods for the matrix logarithm and fractional matrix powers.

I also investigated the effect of structured perturbations on matrix functions. I considered structured matrices comprising either the Jordan algebra $\mathbb{J}$ or the Lie algebra $\mathbb{L}$ associated with a nondegenerate bilinear or sesquilinear form. Structured condition numbers were defined and formulae were given for them. Comparisons were then made between the structured and the unstructured condition numbers. I was able to show that when the underlying scalar product is a sesquilinear form, there is no difference between the values of the two condition numbers for (i) all functions of $X \in \mathbb{J}$, and (ii) odd and even functions of $X \in \mathbb{L}$. When the underlying scalar product is a bilinear form then equality is not guaranteed in all these cases. Where equality is not guaranteed, I have obtained bounds for the ratio of the unstructured and structured condition numbers.

Publications

P. I. Davies and N. J. Higham. Computing $f(A)b$ for Matrix Functions f. Numerical Analysis Report 436, Manchester Centre for Computational Mathematics, Manchester, November 2003. 10 pp. Submitted to the proceedings of the Third International Workshop on Numerical Analysis and Lattice QCD. Edinburgh. 30 June-4 July 2003.

P. I. Davies. Structured Conditioning of Matrix Functions. Numerical Analysis Report 441, Manchester Centre for Computational Mathematics, Manchester, January 2004. 33 pp. To appear in the Electronic Journal of Linear Algebra.

Conferences Presentations

20th Biennial Conference on Numerical Analysis, University of Dundee, June 24-27, 2003. Talk title "Structured Conditioning of Matrix Functions".

New Frontiers in Computational Mathematics Workshop, University of Manchester, January 10-11, 2004. Poster title "Structured Conditioning of Matrix Functions".

Conferences Attended

Third International Workshop on Numerical Analysis and Lattice QCD, Edinburgh, 30 June - 4 July, 2003.

John T. Edwards

Head of Department, University College Chester
Ph.D. University of Birmingham, 1972

I have continued to work on numerical and analytical solutions of integro-differential equations, singular integral equations and various discrete problems. I collaborated with Neville Ford, Jason Roberts, Sophy Thomas and Charles Simpson at Chester on various numerical stability and qualitative analyses for both continuous and discrete problems. I have assisted in the organisation of various seminar days in Chester during 2003. Some of my work was presented at the Dundee Numerical Analysis meeting in June 2003. During his stay as Leverhulme Professor in Chester, I have also begun working with Gennady Bocharov on some problems in mathematical immunology.

Appointments and Professional Activities

Head of Mathematics Department, University College Chester.

Honorary Research Fellow, University of Manchester.

Publications

J.T. Edwards, N.J. Ford and J. A. Roberts. Bifurcations in numerical methods for Volterra integro-differential equations. *International Journal of Bifurcation and Chaos*, 13:3255–3271, 2003.

Judith M. Ford

EPSRC Postdoctoral Research Fellow, UMIST;
Honorary Research Fellow, Chester College
Ph.D. University of Liverpool, 2001

The main focus of my research during 2003 was my project, "Saddle-point systems: is multiresolution analysis the key to effective preconditioning?" in which explored ways of applying wavelet techniques for approximating dense matrices to the solution of saddle-point systems arising from finite element discretization, by sparse approximation of the Schur complement. In this I collaborated with David Silvester and Catherine Powell at UMIST and also had contact with Ke Chen and Stuart Hawkins at Liverpool.

In September I visited the Institute of Numerical Mathematics at the Russian Academy of Sciences in Moscow to continue my colloboration with Eugene Tryrtyshnikov in work on combining wavelet compression with Kronecker product approximation for preconditioning. We developed an algorithm for solving very large dense linear systems relating to functions defined on a two-dimensional grid.

I also published work with Christopher Baker and Neville Ford on some numerical investigations into bifurcations in solutions of Stochastic Delay Differential Equations and contributed to the triennial edition of the Philosophical Transactions of the Royal Society dedicated to the work of outstanding young scientists.

Having been unable to secure permanent employment in a university mathematics department, I left UMIST in January 2004 and am now Research and Development Manager at the Royal Liverpool Children's NHS Trust, Alderhey, Liverpool.

Appointments and Professional Activities

1. Honorary Research Fellow, Chester College.
2. Referee of several articles for academic journals.

Publications

1. J. Ford, K. Chen, and D. Evans. On a recursive Schur preconditioner for iterative solution of a class of dense matrix problems. *Int. J. Comput. Maths.*, 80(1):105–122, 2003.
2. J. Ford and E. E. Tyrtyshnikov. Combining Kronecker product approximation with discrete wavelet transforms to solve dense, function-related linear systems. *SIAM J. Sci. Comput.*, 25(3):961–981, 2003.
3. J. M. Ford, K. Chen and N. J. Ford. Flexible parallelization of fast wavelet transforms. *Parallel Algorithms Appl.*, 18(4):155-169, 2003.
4. J. M. Ford. An improved DWT-based preconditioner for dense matrix problems. *SIAM J. Matrix Anal. Appl.*, 25(3):642-661, 2003.
5. J. M. Ford. A black box at the end of the rainbow: searching for the perfect preconditioner. *Philos. Trans. Royal Soc. Lond. A*, 361(1813): 2665-2680, 2003.
6. C. T. H. Baker, J. Ford, and N. J. Ford. Bifurcations in Approximate Solutions of Stochastic Delay Differential Equations. To appear in *Internat. J. Bifur. Chaos Appl. Sci. Engrg.*, 2003.
7. J. M. Ford, I. V. Oseledets and E. E. Tyrtyshnikov. Matrix Approximations and Solvers using Tensor Products and Non-Standard Wavelet Transforms Related to Irregular Grids. *Russian J. Numer. Anal. Math. Modelling*, 19(2), 2004 (to appear).
8. J. M. Ford, N. J. Ford, and J. Wheeler. Simulation of Grain Boundary Diffusion Creep: Analysis of some New Numerical Techniques. To appear in *Proc. Royal Soc. Lond. A*, 2004.
9. J. M. Ford and J. Wheeler. Modelling interface diffusion creep in 2-phase materials. To appear in *Act Mater.*, 2004.

Presentations

1. March 2003: presented poster at House of Commons reception.
2. May 2003: presented a paper at Quatrième séminaire sur l'algorithmique numérique appliquée aux problèmes industriels, Calais.
3. June 2003: gave contributed talk at NA03 conference, Dundee
4. September 2003: gave invited seminar at Institute of Numerical Mathematics, Russian Academy of Sciences.
5. January 2004: gave contributed talk at New Frontiers in Computational Mathematics conference, Manchester.

Neville J. Ford

Professor of Computational Applied Mathematics, University College Chester;
Honorary Research Fellow, Manchester University
Ph.D. University of Liverpool, 1991

My research continues to focus on numerical and analytical approaches to various classes of functional differential equations. I have recently developed a particular focus on simulations relating to materials with memory through collaboration with scientists at NASA and elsewhere. I lead the Applied Mathematics Research Group at University College Chester, and co-ordinate our programme of international visits and visitors. We have an occasional seminar day programme organised jointly with Christopher Baker.

We have several international co-operations that are current:

with Gennady Bocharov (INMRAS, Moscow) we are developing an active group working on problems in mathematical immunology.

with Teresa Diogo and Pedro Lima (IST, Lisbon) we are working on numerical solutions of some singular integral equations which do not have a unique solution. The work links to the project of Sophy Thomas, a Chester PhD student.

with Sjoerd Verduyn Lunel (Leiden) we continue to work on the detection of small solutions. With my student, Pat Lumb, we have developed a versatile computer software package to detect the presence of small solutions automatically.

with Kai Diethelm and Marc Weilbeer (Braunschweig) and Alan Freed (NASA), I have been developing efficient algorithms for the solution of differential equations of fractional order. Again this is linked to work of a PhD student, Joseph Connolly.

Within the Chester group, I have continued to work with John Edwards and Jason Roberts on bifurcating solutions to integro-differential equations and their discrete analogues. I have also worked with Christopher Baker and Judy Ford on Stochastic Delay Differential Equations (and bifurcating solutions). Finally, I have been working with John Edwards on the qualitative behaviour of Volterra Difference Equations.

I visited Kai Diethelm and Marc Weilbeer (Braunschweig), Gennady Bocharov and Eugenie Tyrtyshnikov (Moscow) and Teresa Diogo and Pedro Lima (Lisbon). I was visited by Wen Chen (Simula Labs, Oslo), Angelina Bijura (Dar es Salaam) and Marc Weilbeer (Braunschweig). I also continued to worked with Alan Freed (NASA) on simulations from materials science.

Appointments and Professional Activities

Director, Applied Mathematics Research Group, University College Chester.

Honorary Research Fellow, University of Manchester.

Director of Chester-Manchester Research Unit on Problems with Memory and After-effect.

Member of EPSRC Peer Review College

Regular Reviewer for Zentralblatt Mathematik and Mathematical Reviews

Publications

J.T. Edwards, N.J. Ford and J.A. Roberts. Bifurcations in numerical methods for Volterra integro-differential equations. *International Journal of Bifurcation and Chaos.* 13, 3255-3271, 2003.

G.A. Bocharov, R.M. Anderson, T. Junt, P. Krebs, B. Metters, N. J. Ford, H. Hengarten, R. M. Zinkernagel and B. Ludewig. Determining the relevant control parameters for dendritic cell-based immunotherapy. *Poster and Abstract, St Gallen.* March 2003.

J. M. Ford, K. Chen and N. J. Ford. Flexible parallelization of fast wavelet transforms. *Parallel Algorithms Appl.*, 18(4):155-169, 2003.

C. T. H. Baker, J. Ford and N. J. Ford. Bifurcations in Approximate Solutions of Stochastic Delay Differential Equations. To appear in *Internat. J. Bifur. Chaos Appl. Sci. Engrg.*, 2003.

J. M. Ford, N. J. Ford, and J. Wheeler. Simulation of Grain Boundary Diffusion Creep: Analysis of some New Numerical Techniques. To appear in *Proc. Royal Soc. Lond. A*, 2004.

Lectures

Invited lecture during visit to the University of Braunschweig (February).

Invited lecture during visit to UTL Lisbon (April).

Invited lecture during visit to INMRAS (Moscow).

I co-organised (with Christopher Baker) various seminar days in Chester.

Lecture at Dundee Numerical Analysis meeting (Plus lectures by my PhD student Pat Lumb and co-worker Teresa Diogo)

Research Grants

I am the host academic for the Leverhulme International Professor Gennady Bocharov who is based in Chester. I received a small grant from the London Mathematical Society to support my collaboration with Teresa Diogo and Pedro Lima in Lisbon.

Nicholas J. Higham

Richardson Professor of Applied Mathematics, University of Manchester
Ph.D. University of Manchester, 1985

2003 was a busy year for conference organization. In my final year as Chair of the SIAM SIAG/LA I was heavily involved in the SIAG's eighth Conference on Applied Linear Algebra, held at the College of William and Mary. The meeting brought together researchers from both the theoretical and applied ends of the subject and attendance increased over the previous meeting. I also helped organize smaller workshops in Germany, at the Schloss Dagstuhl International Conference and Research Center for Computer Science, and Canada, at the Banff International Research Station (BIRS). Both conference centres are remote and provide excellent facilities for research presentations and interaction. The BIRS facility, which opened in March 2003, is the new North American equivalent of Oberwolfach.

One of my main research efforts was focused on "structure-preserving matrix computations", in collaboration with Françoise Tisseur, Niloufer Mackey and Steve Mackey. We considered the matrix sign function and polar decomposition of matrices from automorphism groups $\mathbb{G}$ associated with scalar products. This includes, for example, the complex orthogonal and symplectic groups We identified conditions under which the factors lie in the group and investigated numerical methods that exploit group structure. We have also answered the question "if $A \in \mathbb{G}$ when does $f(A) \in \mathbb{G}$"? The principal matrix square root is such a function and we have derived a new family of square root iterations, some of them structure-preserving.

Many numerical analysis textbooks promulgate the view that the Lagrange interpolation formula is of no practical use, and that the Newton divided difference form should be preferred. Berrut and Trefethen have recently shown the incorrectness of this view, by demonstrating the practical utility of the barycentric form of Lagrange interpolation. One question left open by their analysis is the numerical stability of the barycentric scheme. I have been able to give error analysis to show that the barycentric scheme has excellent numerical stability properties.

During the year I was delighted to take on the editorship of the new SIAM book series *Fundamentals of Algorithms*. The series aims to provide short user-oriented books on state-of-the-art numerical methods, with emphasis on explaining how to best choose a method, algorithm or software to solve a specific type of problem, and describing when a given method works or fails. I have been able to as-

semble a distinguished editorial board and we are busy soliciting manuscripts from potential authors.

Finally, I was honoured to be awarded a Royal Society-Wolfson Research Merit Award, having been nominated for it by the VC of the University, Sir Martin Harris. The new School of Mathematics will be unique among Mathematics departments in having two Award holders amongst its members, the other being Professor Martin Taylor, FRS.

Appointments and Professional Activities

Director of Manchester Centre for Computational Mathematics.

Head of Numerical Analysis Group.

Director of M.Sc. in Applied Numerical Computing.

Chair of Departmental Research Committee.

Member of Executive Committee of the Centre for Novel Computing in the Department of Computer Science, University of Manchester.

(Founding) Editor-in-Chief of SIAM Fundamentals of Algorithms book series,

Editorial board, SIAM Journal on Matrix Analysis and Applications.

Editorial board, IMA Journal of Numerical Analysis.

Editorial board, Linear Algebra and Applications.

Editorial board, Foundations of Computational Mathematics.

Editorial board, Numerical Algorithms

Editorial board, SIAM News.

Member of Executive Committee of Foundations of Computational Mathematics.

Member of EPSRC Peer Review College.

Chair of the SIAM Activity Group on Linear Algebra.

Member of organizing committee of Householder Symposia.

Member of organizing committee of Eighth SIAM Conference on Applied Linear Algebra, College of William and Mary, Williamsburg, July 2003.

Organizer, with Dr F. Tisseur, Dr T. Shardlow and Prof. D. J. Silvester, of 2-day workshop "New Frontiers in Computational Mathematics", University of Manchester, January 2004.

Publications

(These publications are available from my Web page at `http://www.ma.man.ac.uk/~higham/`)

A. Bojanczyk, N. J. Higham, and H. Patel. The equality constrained indefinite least squares problem: Theory and algorithms. *BIT*, 43(3):505–517, 2003.

A. Bojanczyk, N. J. Higham, and H. Patel. Solving the indefinite least squares problem by hyperbolic QR factorization. *SIAM J. Matrix Anal. Appl.*, 24 (4):914–931, 2003.

P. I. Davies and N. J. Higham. Computing $f(A)b$ for matrix functions f. Numerical Analysis Report No. 436, Manchester Centre for Computational Mathematics, Manchester, England, Nov. 2003. 10 pp. Submitted to Proceedings of the Third International Workshop on QCD and Numerical Analysis, Edinburgh, 2003.

P. I. Davies and N. J. Higham. A Schur–Parlett algorithm for computing matrix functions. *SIAM J. Matrix Anal. Appl.*, 25(2):464–485, 2003.

N. J. Higham. J-orthogonal matrices: Properties and generation. *SIAM Rev.*, 45(3):504–519, Sept. 2003.

N. J. Higham. The numerical stability of barycentric Lagrange interpolation. Numerical Analysis Report No. 440, Manchester Centre for Computational Mathematics, Manchester, England, Dec. 2003. 10 pp. Revised January 2004. To appear in IMA J. Numer. Anal.

N. J. Higham. SIAG/LA prizewinners speed up the QR algorithm. *SIAM News*, 36(9):3, Nov. 2003.

N. J. Higham, M. Konstantinov, V. Mehrmann, and P. Petkov. Sensitivity of computational control problems. Preprint 2003/5, Institut für Mathematik, TU Berlin, D-10623 Berlin, FRG, 2003.

N. J. Higham, D. S. Mackey, N. Mackey, and F. Tisseur. Computing the polar decomposition and the matrix sign decomposition in matrix groups. Numerical Analysis Report No. 426, Manchester Centre for Computational Mathematics, Manchester, England, Apr. 2003. 16 pp. Revised November 2003. To appear in SIAM J. Matrix Anal. Appl.

N. J. Higham and M. I. Smith. Computing the matrix cosine. *Numerical Algorithms*, 34:13–26, 2003.

N. J. Higham and F. Tisseur. Bounds for eigenvalues of matrix polynomials. *Linear Algebra Appl.*, 358:5–22, 2003.

Lectures

Spectral Theory Network Conference IV, University of Edinburgh, June 2003. "Matrix Functions: Theory and Algorithms".

20th Dundee Biennial Conference on Numerical Analysis, June 2003. "Computing the Polar Decomposition in Matrix Groups".

Third International Workshop on Numerical Analysis and Lattice QCD, e-Science Institute, Edinburgh, July 2003. "Matrix Functions: Theory and Algorithms".

Eighth SIAM Conference on Applied Linear Algebra, College of William and Mary, Williamsburg, July 2003. "J-Orthogonal Matrices: Properties and Generation".

28th Conference of the Dutch-Flemish Numerical Analysis Communities, Woudschoten Conference Centre, Zeist, The Netherlands, October 2003. Two lectures on "Matrix Functions: Theory, Algorithms and Software".

Theoretical and Computational Aspects of Matrix Algorithms Workshop, Schloss Dagstuhl International Conference and Research Center for Computer Science, Germany, October 2003. "Structure-Preserving Iterations on Matrix Groups".

Workshop on Theory and Numerics of Matrix Eigenvalue Problems, Banff International Research Station, Canada, November 2003. "Matrix Functions Preserving Group Structure and Iterations for the Matrix Square Root".

Dept of Mathematics and Statistics, University of Calgary, November 2003. "Functions of a Matrix: Theory, Applications and Algorithms".

Research Grants

Principal investigator on project "Numerical Analysis of Matrix Functions" funded by EPSRC Mathematics Committee for three years from February 2001 (value £129,092). Grant GR/R22612.

Principal investigator on Masters Training Package "Applied Numerical Computing" funded by EPSRC for five years from April 2002 (value £564,602). Co-investigator Prof. D. J. Silvester. Grant GR/R59984/01.

For 2-day workshop "New Frontiers in Computational Mathematics" held in January 2004 at the University of Manchester:

- Grant of £6500 from the University of Manchester,
- Grant of £1200 from London Mathematical Society.

Co-investigator (PI Dr. F. Tisseur) on EPSRC Visiting Fellowship for Professor N. Mackey (W. Michigan University) on project "Structured Eigenvalue Problems: Theory and Numerics", September 2002–April 2003. Grant GR/S15563/01 (value £9958).

Co-investigator (PI Dr. F. Tisseur) on EPSRC grant "Model Compaction and Model Reduction Methods for Large-Scale Dynamic Systems in Engineering" (value £132,498) funded by Computational Engineering Mathematics (6th call) for three years from October 2003. Grant GR/S31693/01.

Royal Society-Wolfson Research Merit Award holder, 2003–2008, £175,000.

Catherine Elizabeth Powell

Temporary Lecturer in Applied Mathematics.
Ph.D. UMIST, November 2003.

I joined the mathematics department at UMIST in September on a temporary three-year contract as Lecturer in Applied Mathematics. This coincided with the submission of my Ph.D thesis, which I successfully defended in November 2003.

My research interests are centered on aspects of numerical linear algebra in the context of solving algebraic systems of equations derived from discretisations of PDEs. My current research is mainly concerned with preconditioning methods for saddle-point systems. In particular, I am investigating and developing fast and robust solution methods for those systems derived from mixed finite element formulations of Darcy flow. I am also involved in a research project with postdocs at UMIST investigating the efficiency of algebraic multigrid as a solver for a forward problem arising in electrical resistance tomography.

In 2004, I plan to investigate aspects of numerical linear algebra associated with stochastic models of groundwater flow.

Publications

C. E. Powell. Optimal preconditioning for mixed finite element formulation of second-order elliptic problems. *Ph.D thesis,* UMIST, November 2003.

C. E. Powell and D. Silvester. Optimal preconditioning for Raviart-Thomas mixed formulation of second-order elliptic problems. *SIAM J. Matrix Anal. Appl.,* vol 25, no. 3, pp.718–738, 2003.

C. E. Powell and D. Silvester. Black-box preconditioning for mixed formulation of self-adjoint elliptic PDEs. *Lect. Notes Comput. Sci. Eng.,* 35, 2003.

Christopher A. H. Paul

Research Fellow/Computer Support, Officer/Procurement Officer, University of Manchester
PhD. University of Manchester, 1992

Appointments and Professional Activities

Computer Support Officer, Department of Mathematics.

Procurement Officer, Department of Mathematics.

Chair of the Faculty of Science & Engineering Computer Components Procurement subgroup.

Member of the University Computer Working Strategy Group.

Referee for Journal of Computational and Applied Mathematics.

Member of EPSRC College 2003 onwards.

Publications

Christopher T. H. Baker, Gennadii A. Bocharov, Christopher A. H. Paul, and Fathalla A. Rihan. Models with delays for cell population dynamics: Identification, selection and analysis. part i: Computational modelling with functional differential equations: Identification, selection, and sensitivity. Numerical Analysis Report No. 425, Manchester Centre for Computational Mathematics, Manchester, England, February 2003. 28 pp.

Christopher T. H. Baker and Christopher A. H. Paul. Piecewise continuous solutions of neutral delay differential equations. Numerical Analysis Report No. 417, Manchester Centre for Computational Mathematics, Manchester, England, December 2003. 35 pp.

J. A. Roberts

Assistant, Mathematics Department, University College Chester
Ph.D. Liverpool University, 2000

I am continuing my work on stability and bifurcations in numerical solutions of integral and integro-differential equations. I have begun work on stochastic integro-differential equations (stability and numerical stability) and am collaborating with Leonid Shaikhet from the Ukraine in this project.

Publications

J T Edwards, N J Ford and J A Roberts. Bifurcations in numerical methods for Volterra integro-differential equations. *International Journal of Bifurcation and Chaos.* 13, 3255-3271, 2003.

Research Grants

I received a research grant from the NATO Science Programme to support a collaborative research project with Professor Leonid Shaikhet from Donetsk SAM, Ukraine.

Tony Shardlow

Lecturer
Ph.D. Stanford, 1997

My research interests are centered on stochastic differential equations, where I have a number of active projects. I am interested in simulating and analysing stochastic PDEs that model excitable media. With postdoc Yubin Yan, we are investigating Dissipative Particle Dynamics, a system of stochastic differential equations that model multiphase fluid flows. With my collaborators in Germany Evelyn Buckwar and Hagen Gilsing, we are developing a software package to simulate stochastic differential equations.

In addition to this line of work, I recently developed an interest in numerical optimisation and its applications in image analysis. With Ph.D. student Anna Mills and collaborator Stephen Marsland, we are developing algorithms to register medical images using the geodesic interpolating spline. Anna Mills recently won a Cecil King Scholarship to work on this project for three months at Massey University New Zealand with Stephen Marsland.

Research Grants

Principal Investigator on project "Implicit Methods for Dissipative Particle Dynamics, EPSRC, funding postdoc Yubin Yan.

Support to attend LMS summer school on Markov Chains, July 03.

Publications

Tony Shardlow. Splitting for dissipative particle dynamics. *SIAM Journal on Scientific Computing*, 24 (4):1267–1282, July 2003.

Tony Shardlow, Weak convergence of a numerical method for a stochastic heat equations *BIT* 43: 179–193, 2003

Blowey, J. F., Craig, A. W., and Shardlow, T., eds, Frontiers in Numerical Analysis, Springer, 2003.

Shardlow, T. and Buckwar, E. Weak approximation of stochastic differential delay equations, *IMAJNA*, to appear. NA Report 439.

Shardlow, T. Nucleation of waves in excitable media by noise, NA Report 438.

Shardlow, T. Numerical simulation of stochastic PDEs for excitable media, NA Report 437.

Lectures

"Dissipative Particle Dynamics," Dundee, June 2003.

MIRW day "Multiscale analysis for Stochastic Dynamics" Warwick, October 2003.

Stochastic PDE Conference, Warwick, July 2003.

SciCADE minisymposium on Computational Stochastic PDE, Trondheim, July 2003.

David J. Silvester

Professor
Ph.D. University of Manchester, 1984

My research effort continues to revolve around writing a research textbook: *Finite Elements and Fast Iterative Solvers*, to be published by Oxford University Press in the Numerical Mathematics and Scientific Computation Series. This is a joint project with two collaborators; Professor Howard Elman (University of Maryland) and Dr Andy Wathen (Oxford University Computing Laboratory). We expect to finish writing the book over the Summer (finally!), and we anticipate publication before the end of 2004.

I had a six month period of study leave between February and July. In January and February I was a long stay visitor at the Newton Institute programme on *Computational Challenges in Partial Differential Equations*. I also spent five weeks at the University of Maryland visiting Professor Elman. During this visit, I was an invited speaker at a *Workshop on Perspectives on Incompressible Flows,* hosted by the Institute for Scientific Computing at the University of Maryland, and organised by Professor Eitan Tadmor. I was also invited to a workshop on *Mathematical Aspects of Computational Fluid Dynamics* at the Oberwolfach Institute in November, and to a workshop on *Saddle-point Problems* held in Santa Fe in December.

My research student Catherine Powell successfully submitted her Ph.D thesis on "Optimal Preconditioning for Mixed Finite Element Formulation of Second-Order Elliptic Problems" in September. She took up the position of a lecturer in the department at the end of September (see her separate entry).

Research avenues that I am actively exploring at present include: groundwater flow modelling (with Catherine Powell); stability of mixed finite elements on stretched grids (with Professor Mark Ainsworth from the University of Strathclyde); anisotropic mesh refinement (with my PhD student Nick Watson, and Dr David Kay from the University of Sussex); and adaptivity for the Navier-Stokes equations (with David Kay, Dr David Griffiths and Dr Philip Gresho, latterly an EPSRC visiting fellow at UMIST).

Other project proposals currently being prepared or being considered by the EPSRC that I plan to contribute to include: Black-box solver software for high performance computers (with Dr Milan Mihajlovic and Dr Jennifer Scott); and fluid-structure interaction in modelling lung-biomechanics (with Dr Matthias Heil).

Professional Activities

Editorial board, SIAM Journal on Scientific Computing.

Editorial board, International Journal for Numerical Methods in Fluids.

Member of EPSRC Peer Review College 2000–present.

Research Grants

LMS Scheme 4 grant to collaborate with Professor Elman. Grant 4819 (value £500).

Investigator on MTP project "Applied Numerical Computing", EPSRC funded M.Sc programme, April 2002—September 2007. Grant GR/R59984/01 (value £565,000).

Publications

All of these publications are available via the WWW, see `http://www.ma.umist.ac.uk/djs/`

C. E. Powell and D. Silvester. Optimal preconditioning for Raviart-Thomas mixed formulation of second-order elliptic problems. *SIAM J. Matrix Anal. Appl.,* vol 25, no. 3, pp.718–738, 2003.

Powell, C and Silvester, D., Black-box preconditioning for mixed formulation of self-adjoint elliptic PDEs, *Challenges in Scientific Computing — CISC 2002.* Bänsch E. (Ed), Springer Lecture Notes in Computational Science and Engineering **35**, pp. 268–285, 2003.

Syamsudhuha and Silvester, D. Efficient solution of the steady-state Navier-Stokes equations using a multigrid preconditioned Newton-Krylov method, Int. J. Numerical Methods in Fluids, **43**, pp. 1407–1427, 2003.

Lectures

Seminar at the Newton Institute, Cambridge, February 2004.

Invited speaker at a *Workshop on Perspectives on Incompressible Flows,* held at the Institute for Scientific Computing, College Park, USA, April 2004. All expenses paid by the organisers.

Seminar at the Mathematics Department, University of Maryland, USA, April 2004.

Invited speaker at a *Workshop on the Mathematical Aspects of Computational Fluid Dynamics* at the Mathematisches Forchungsinstitut Oberwolfach, Germany, November 2004. All local expenses paid by the organisers.

R. W. Thatcher

Senior Lecturer
Ph.D. University of London, 1972

I have continued to work on least squares techniques for fluid flow in collaboration with a former research student, Paul Bolton. Paul has submitted a joint paper concerning the importance of mass conservation and is writing a second paper on extending our stress/stream function approach to modelling the Navier Stokes equations. We have also begun to extend our ideas to three dimensional flows.

My main area of research over the last twelve months has continued to be concerned with Numerical Modelling in Combustion. Much of the recent work has been concerned with modelling the edges of flames, concentrating on the stability of solutions and flame edges at non-unit Lewis Numbers. The work on flame edges has been carried out with Alessandro Omon-Arancibia, a student jointly with John Dold. A second research student, Eman Al-Sarairah, is working on flame edges in the presence of heatloss, a project in collaboration with Joel Daou.

Appointments and Professional Activities

Head of the Mathematics Department, UMIST.

Publications

Flame balls with thermally sensitive intermediate kinetics, (with J. W. Dold, R. O. Webber and A. A. Shah), Combustion Theory and Modelling **7** (2003), 175-203.

Multiple speeds of triple flame propagation at Lewis numbers above one, (with A. A. Omon-Arancibia), submitted to Combustion Theory and Modelling.

On mass conservation in least squares methods, (with P. Bolton), submitted to Journal of Computational Physics.

Ruth M. Thomas

Senior Lecturer
Ph.D. University of Manchester, 1979

In 2003, I worked on two main research projects. The first project concerns the numerical solution of periodic initial value problems with oscillatory solution. I collaborated with Dr. John Coleman of the University of Durham and with a Ph.D. student, Paul Roberts, on developing collocation methods for solving problems of this type.

In the second project, I worked on moving mesh methods for parabolic partial differential equations, in particular for problems arising when modelling the propagation of a narrow flame in a detonator delay element. This work was in collaboration with Dr. Thebe Basebi of the University of Botswana.

Appointments and Professional Activities

External Examiner, M.Sc. Course in Computational Mathematics and Modelling, University of Brunel.

Referee of numerous papers for academic journals.

Referee of several research proposals for the EPSRC.

Departmental responsibilities include being Assistant Head of Department, Director of Undergraduate Studies and Undergraduate Tutor.

Publications

T. Basebi and R. M. Thomas. A Study of Moving Mesh Methods Applied to a Thin Flame Propagating in a Detonator Delay Element. *Computers and Mathematics with Applications*, **45**, 131-163 (2003).

Françoise Tisseur

Colin Roscoe Lecturer in Numerical Analysis
Ph.D. University of St. Etienne, 1997

Over the last year, I continued my work on structured matrices and generalized and polynomial eigenvalue problems. I was on maternity leave from April until October.

In collaboration with Niloufer Mackey and Steve Mackey (Western Michigan University) we continued our work on structured matrices belonging to automorphism groups $\mathbb{G}$ associated with a scalar product. This include for examples the complex orthogonal, pseudo-orthogonal and symplectic groups. We characterized analogues of Householder transformations in $\mathbb{G}$ and called them $\mathbb{G}$-reflectors. To our knowledge, this is the first time these transformations, together with their mapping properties, have all been presented under a common rubric and developed from a constructive matrix perspective. This work should stimulate further investigations, both theoretical and algorithmic, where the preservation of structure is desired.

With Nick Higham, Niloufer Mackey and Steve Mackey we also considered matrix sign function and polar decomposition in $\mathbb{G}$. We showed that the polar factors of $A \in \mathbb{G}$ lie in $\mathbb{G}$ if the matrix of the underlying scalar product is unitary. We investigated several numerical methods that exploit group structure.

As part of my effort to investigate the numerical solution of symmetric indefinite generalized eigenvalue problems, I derived with Dario Bini and Luca Gemignani (University of Pisa) a new algorithm for the tridiagonal–diagonal eigenvalue problem that is faster than the LAPACK subroutine `dhseqr` for large dimensions and more accurately approximates eigenvalues with small moduli.

In April, I was awarded an EPSRC grant for three years to work on "Model Compaction and Model Reduction Methods for Large-Scale Dynamic Systems in Engineering". Steve Mackey was appointed in September as research associate to work on this project.

Professional Activities

Organizer of minisymposium "Numerical Solution of Polynomial Eigenvalue Problems", Eighth SIAM Conference on Applied Linear Algebra, Williamsburg, Virginia, July 2003.

Organizer, with Professor N. J. Higham, Dr T. Shardlow and Professor D. J. Silvester of 2-day workshop "New Frontiers in Computational Mathematics", University of Manchester, 2004.

Publications

(These publications are available from my Web page at `http://www.ma.man.ac.uk/~ftisseur/`)

N. J. Higham and F. Tisseur. Bounds for Eigenvalues of Matrix Polynomials. *Linear Algebra and Appl.*, 358:5-22, 2003.

J.-P. Dedieu and F. Tisseur. Perturbation Theory for Homogeneous Polynomial Eigenvalue Problems. *Linear Algebra and Appl.*, 358:71–94, 2003.

J.-P. Dedieu, M.-H. Kim, M. Shub and F. Tisseur. Implicit Gamma Theorems (I): Pseudoroots and Pseudospectra. *Foundations of Comp. Math.*, 3:1–31, 2003.

F. Tisseur. A Chart of Backward Errors and Condition Numbers for Singly and Doubly Structured Eigenvalue Problems, *SIAM J. Matrix Anal. Appl.*, 24(3):877–897, 2003.

S. D. Garvey, F. Tisseur, M. I. Friswell and J. E. T. Penny. Simultaneous Tridiagonalization of Two Symmetric Matrices, *Int. J. Numer. Meth. Engng.*, 57(12):1643–1660, 2003.

D. S. Mackey, N. Mackey and F. Tisseur. Structured Tools for Structured Matrices. *The Electronic Journal of Linear Algebra*, (10):106–145, 2003.

D. S. Mackey, N. Mackey and F. Tisseur. $\mathbb{G}$-Reflectors: Analogues of Householder Transformations in Scalar Product Spaces. Numerical Analysis Report 420, Manchester Centre for Computational Mathematics, February 2003. *To appear in Linear Algebra and its Applications.*

N. J. Higham, D. S. Mackey, N. Mackey and F. Tisseur. Computing the Polar Decomposition and the Matrix Sign Decomposition on Matrix Groups; Numerical Analysis Report 426, Manchester Centre for Computational Mathematics, April 2003. *To appear in SIAM J. Matrix Anal. Appl.*.

D. Bini, L. Geminiani and F. Tisseur. The Ehrlich-Aberth Method for the Nonsymmetric Tridiagonal Eigenvalue Problem; Numerical Analysis Report 428, Manchester Centre for Computational Mathematics, June 2003.

Lectures

20th Dundee Biennial Conference on Numerical Analysis, June 2003. "Solving Symmetric Quadratic Eigenvalue Problems".

Workshop "Theory and Numerics of Matrix Eigenvalue Problems", *Banff International Research Station*, Canada, November 2003. *Attendance by invitation only.*

Research Grants

Award to Newly Appointed Lecturers in Science, Engineering and Mathematics from the Nuffield Foundation. Amount of grant: £4,845 (maximum award is £5K), 2001–2003. Grant Number: NAL/00216/G.

Principal Investigator on project "Numerical Analysis of Polynomial Eigenvalue Problems" funded by EPSRC Mathematics Committee under the "Fast Stream" scheme for three years from September 2001 (value £62,553). Grant GR/R45079/01.

Principal Investigator on EPSRC Visiting Fellowship for Prof. N. Mackey (W. Michigan University) on project "Structured Eigenvalue Problems: Theory and Numerics", Sept 2002–April 2003. Grant GR/S15563/01 (value £9958).

Principal Investigator on project "Model Compaction and Model Reduction Methods for Large-Scale Dynamic Systems in Engineering" funded by EPSRC under the Computational Engineering Mathematics scheme (6th call) for three years form September 2003 (value £132,498). Grant GR/S31693/01.

Yubin Yan

Research associate
Ph.D. Chalmers, Gothenburg, 2003

I got my PhD in mathematics in Chalmers University of Technology (Sweden) in June 2003. Soon after, I came to the University of Manchester as a research associate. I am now working on the project " Implicit Methods for Dissipative Particle Dynamics" funded by EPSRC. Together with Dr. Tony Shardlow we try to develop a new mathematical method to understand the geometric ergodicity of dissipative particle dynamics, a system of stochastic differential equations that model multi-phase fluid flows.

Professional Activities

Referee for "Journal of Computational Physics", "Applied Mathematics and Computation".

Publications

Yubin Yan. Smoothing properties and approximation of time derivatives for parabolic equations: variable time steps. *BIT* 43:647–669, 2003.

Yubin Yan. Smoothing properties and approximation of time derivatives for parabolic equations: constant time steps. *IMA J. Numer. Anal.*, 23:465–487, 2003.

Yubin Yan. Postprocessing the finite element method for semilinear parabolic problems. Preprint 2003–06, Chalmers Finite Element Center, Chalmers University of Technology. To appear in *SIAM Journal of Numerical Analysis*.

Lectures

Workshop on Stochastic Partial Differential Equations and Related Topics , Warwick, UK, August 4 - August 15, 2003, (20 minutes talk)

3 Long-Term Visitors

Rafikul Alam

Associate Professor
Indian Institute of Technology Guwahati
Ph.D. Indian Institute of Technology Bombay, 1996

Over the year I worked on application of ϵ-pseudospectra in analyzing sensitivity of eigenvalues and eigendecompositions of matrices. Also, for the semester January-April, 2003, I taught an advanced analysis course to Post Graduate students at the Department of Mathematics, Indian Institute of Technology Guwahati.

From March 25, 2003, to March 21, 2004, I visited Professor Nick Higham and Dr Françoise Tisseur at the Department of Mathematics, University of Manchester, supported by the Department of Science & Technology, Govt. of India, in the form of a BOYSCAST fellowship. During the visit we worked on a problem due to Wilkinson which has been unsolved for nearly forty years. Given an n-by-n matrix with n distinct eigenvalues, the problem concerns finding the nearest defective matrices. We have investigated theoretical and computational issues related to Wilkinson's problem.

From February 4-11, 2004, I visited Professor Volker Mehrmann at the Department of Mathematics, TU-Berlin, Germany. During my visited I worked with Professor Ralph Byers, Dr. Shreemayee Bora and Professor Michael Overton towards developing a practical algorithm for computing the nearest defective matrices.

Also, I continued to write reviews for the Mathematical Reviews published by the American Mathematical Society.

Publications

1. R. Alam and S. Bora, On ϵ-spectral analysis of matrices, *International Workshop on Linear Algebra, Numerical Functional Analysis and Wavelets Analysis,* S.H. Kulkarni and M.N.N. Namboodiri, eds., pp.25-44, Allied Publishers, Chennai, 2003.

2. R. Alam. On the construction of nearest defective matrices to a normal matrix, Numerical Analysis Report 433, Manchester Centre for Computational Mathematics, September, 2003.

3. R. Alam and N. J. Higham. On the construction of a nearest defective matrix, to be published as an MCCM NA Report.

4. R. Alam, S. Bora, R. Byers and M. Overton, An algorithm for computing a nearest defec-

tive matrix, in preparation, to be published as a Tech. Report of TU-Berlin, Germany.

Lectures

1. "A simple guaranteed algorithm for computing the distance to the nearest defective matrices", Institüt fur Mathematik, TU-Berlin, February, 2004.

2. "Computing stable eigendecompositions of matrices", Department of Mathematics, University of Manchester, December, 2003.

Workshops/Conferences attended

1. 20th Biennial Conference on Numerical Analysis, University of Dundee, June 24-27, 2003.

2. Spectral Theory Network Conference IV, University of Edinburgh, June 23-25, 2003.

3. New Frontiers in Computational Mathematics Workshop, University of Manchester, January 10-11, 2004.

Sven Hammarling

Simon Industrial and Professional Fellow, University of Manchester
NAG Ltd, Oxford

Due to illness, I was unable to complete the Fellowship during the academic year, but the University kindly allowed the remaining three weeks of the Fellowship to be carried over. Nevertheless, I was able to give lectures to the students on the MSc in Applied Numerical Computing, to collaborate with Craig Lucas on his PhD studies, particularly in the area of block partitioned algorithms for pivoted Cholesky factorization and for updating QR factorizations, and to complete work on updating some of the LAPACK least squares solvers. A number of useful discussions were held with members of both the Departments of Mathematics and of Computer Science (the Fellowship is joint with both departments).

Niloufer Mackey

Associate Professor, Western Michigan University
Ph.D. State University of New York at Buffalo, 1995

I continued my sabbatical visit with Professor Nick Higham and Dr Françoise Tisseur. This visit, for the period September 2002 through early April 2003 was supported by an EPSRC Visiting Fellowship. I returned to the University of Manchester for about two weeks in December, to continue the collaboration with Higham and Tisseur.

Together with D. S. Mackey, we tackled a wide range of problems related to structured matrices. We developed an extensive collection of structure-preserving transformations that perform the basic actions on which the majority of the algorithms of numerical linear algebra rely. The notion of Householder transformations was extended to scalar product spaces, giving a complete characterization of these transformations and their mapping properties for a large class of automorphism groups. We investigated the existence of structured versions of several important matrix factorizations, and built structure-preserving iterations for the matrix sign function, the polar decomposition and the principal square root.

We also investigated two mapping problems: given a class of structured matrices $\mathbb{S}$, determine for which pairs of vectors x, b, there is a linear mapping $A \in \mathbb{S}$ such that $Ax = b$, and characterize the set of all such $A \in \mathbb{S}$. We have solved these problems when $\mathbb{S}$ is the automorphism group or the Lie or Jordan algebra associated with an orthosymmetric scalar product. These results are part of a working manuscript.

With D. S. Mackey, a collection of old and new proofs showing that the determinant of a symplectic matrix is always $+1$ was put together. Structured factorizations of symplectic matrices played a key role in several arguments. A constructive derivation of the symplectic analogue of the Cartan-Dieudonné theorem is one of the new proofs in the essay.

Work on canonical forms and structure-preserving algorithms for solving the complete eigenproblem for matrices that are either symmetric or skew-symmetric about the main diagonal as well as the antidiagonal was completed. These algorithms exhibit greater numerical stability, and are likely to be strongly backward stable. Because they are Jacobi-like, they are readily adaptable for parallel computation.

Publications

D. S. Mackey, N. Mackey and F. Tisseur. Structured Tools for Structured Matrices. *The Electronic Journal of Linear Algebra*, (10):106–145, 2003.

D. S. Mackey, N. Mackey and F. Tisseur. $\mathbb{G}$-Reflectors: Analogues of Householder Transformations in Scalar Product Spaces. Numerical Analysis Report 420, Manchester Centre for Computational Mathematics, February 2003. *To appear in Linear Algebra and its Applications.*

D. S. Mackey and N. Mackey. On the determinant of symplectic matrices. Numerical Analysis Report

422, Manchester Centre for Computational Mathematics, February 2003.

N. J. Higham, D. S. Mackey, N. Mackey and F. Tisseur. Computing the Polar Decomposition and the Matrix Sign Decomposition on Matrix Groups; Numerical Analysis Report 426, Manchester Centre for Computational Mathematics, April 2003. Revised November 2003. *To appear in SIAM J. Matrix Anal. Appl.*.

D. S. Mackey, N. Mackey, and D. M. Dunlavy. Structure preserving algorithms for perplectic eigenproblems. Numerical Analysis Report 427, Manchester Centre for Computational Mathematics, May 2003. Submitted to *The Electronic Journal of Linear Algebra.*

Lectures

Numerical Analysis Seminars, Department of Applied Mathematics and Theoretical Physics, Cambridge University, England. March 6, 2003. "Spectral Effects with Quaternions".

Oberseminar Numerik, Technische Universität Berlin, Germany. April 22, 2003. "Spectral Effects with Quaternions".

Mathematischen Kolloquiums, Technische Universität Braunschweig, Braunschweig, Germany. July 1, 2003. "Factorizations in Matrix Groups".

Oberseminar Numerik, Universität Bielefeld, Bielefeld, Germany. July 3, 2003. "Factorizations in Matrix Groups".

Eighth SIAM Conference on Applied Linear Algebra, College of William and Mary, Williamsburg, USA. July 2003. "$\mathbb{G}$-Reflectors in Scalar Product Spaces".

Theory and Numerics of Matrix Eigenvalue Problems, Banff International Research Station, Banff, Canada. November 2003. "Structured Tools and Factorizations in Scalar Product Spaces".

4 Numerical Analysis at the University of Manchester, 1957–1979

The development of Numerical Analysis in Manchester was stimulated by the pioneering work on automatic computers which started in Manchester in the late 1940's. The research group on computers was led by F.C. Williams and T. Kilburn in the Department of Electrical Engineering; the Manchester Mark 1 machine came into operation in 1948, followed by the Mark 2 (prototype Mercury) in 1954 and the Atlas in 1962. At the same time the Mathematics Department was expanding considerably under Max Newman, Sydney Goldstein and James Lighthill. Newman was a strong supporter of the computing project, foreseeing its importance for many areas of mathematics as well as for other fields. In 1957 he appointed Dr C. B. Haselgrove (who had been working on the first computer at Cambridge) to promote research in mathematical computing in Manchester. Some of the applications of computers were immediately obvious; many well-formulated problems in science and engineering which required numerical solutions could benefit directly from faster computation. This was particularly true in astronomy, a classical area for numerical work, where the research at Jodrell Bank called for major computing support. But there was also the prospect of using automatic machines to solve analytical and logical problems in new ways, which were not simply accelerated versions of existing methods

Brian Haselgrove's research interests ranged over many areas of mathematics both pure and applied. At Cambridge he had collaborated with J. C. P. Miller on table- making (for the Riemann zeta function), and at Manchester he published papers on Dirichlet functions and the Riemann hypothesis, ray paths in the ionosphere, numerical integration using quasi-random numbers, two-point boundary-value problems, and some geometrical puzzles. The paper on boundary-value problems (*Comp. J.*, 4. 1962, p. 255) illustrates an early stage of what was to become a major interest of numerical analysts at Manchester and elsewhere, the development of general algorithms. This work involves the elucidation of classes of mathematical problems which are suitable for solution by a standardised approach. The solution methods have to be studied analytically and tested on an extensive range of problems, to determine their applicability and limitations. In the early 1960's the potential for general solvers was becoming apparent, but the programming languages available did not provide enough flexibility for implementation.

On the teaching side, Haselgrove initiated a postgraduate Diploma in Computing in 1959 in collaboration with Tony Brooker and other members of the Computing group. In 1964 Computer Science became a separate Department, and the postgraduate course (which became an M.Sc. in 1965) began to concentrate on the more mathematical aspects of computing, retaining some options from Computer Science. Student numbers were relatively small at first, but the course provided a source of research students in Numerical Analysis. Haselgrove also introduced an undergraduate course in numerical methods and computer programming, but it was not possible to include realistic practical work until autocodes were designed.

The Department supported the expansion of activity in numerical mathematics by providing further posts in the 1960's. Joan Walsh was appointed from CEGB in April 1963, and Geoffrey Shearing and Will McLewin (who were already in Manchester) in October 1963. Brian Haselgrove died after a short illness in 1964. The group began to arrange short courses on effective numerical computation for users across the university, with the help of colleagues from Physics, Engineering, and Computation at UMIST. It was soon evident that widespread use of the computer by non-specialists would require the "packaging" of mathematical expertise into easily-applied programs, and contacts with users showed the main areas of demand. A prime mover in this direction was J. H. Wilkinson at the National Physical Laboratory, who produced highly developed methods for many basic problems of linear algebra. Another requirement among chemists and physicists was the accurate computation of special functions, which created a minor industry in the area of Chebyshev approximation. These and other advances in mathematical computation were brought together at an IMA conference in Birmingham in 1965, which attracted a large audience and promoted the value of good mathematical methods in numerical work.

The range of topics covered by the Manchester group was broadened by additional appointments: George Hall in 1965, Christopher Baker in 1966, and Ian Gladwell in 1969. (Geoffrey Shearing had earlier moved to Newcastle.) At this time the main users of numerical computation were scientists and engineers; applied mathematicians had a strong tradition of pursuing their problems by classical analysis as far as possible, and resorting to the computer only when all else failed. But many problems in science and engineering were quite intractable without computers, and large-scale numerical modelling of physical situations became feasible and popular as machines became more powerful. Leslie Fox (then at Oxford) was con-

cerned that basic mathematical research in Numerical Analysis should not be neglected, and he advocated a special initiative by the Science Research Council (now EPSRC) to encourage greater research activity in the theory of numerical computation. The SRC eventually made special grants in the early 1970's to three institutions (Oxford, Dundee and Manchester), to strengthen their research groups by supporting research students, fellows and visitors. This helped to raise the profile of the subject, and to improve links with overseas workers, particularly in the U.S.

When standard computer languages were introduced in the 1960's, it became possible to address the need for high-quality algorithms. In linear algebra, where the problems were relatively easy to classify, a series of Algol procedures were published by Wilkinson and others in the journal *Numerische Mathematik*, and collected into a Handbook in 1971. This material then had to be implemented on particular computers, and translated into Fortran for general use. Wider distribution showed that difficulties could arise from variable word-lengths and computer arithmetic, and that strict language standards were needed. In 1970 a group of institutions which had common computing hardware (ICL 1906A machines) agreed to form a consortium to work on a library of algorithms, the original members being Nottingham, Leeds, Oxford, Birmingham, Manchester and the Atlas Laboratory at Chilton. The aim was to collaborate in the development of a comprehensive mathematical library, with high standards of testing, documentation, and maintenance. The first edition of the library was issued in Sept 1971, and within a few years, by careful attention to word-length problems and language variations, it became possible to make it available for most machine ranges. The consortium attracted support from many academic and research groups, and it was incorporated as the Numerical Algorithms Group (NAG Ltd) in 1976. The Manchester group was involved in the NAG project from the beginning, providing contributors, testers, and validators. A particularly significant contribution was made by Ian Gladwell, in the section on ordinary differential equations. The project received financial help from the Computer Board (a Government agency) for several years, until it was able to support itself by commercial sales of the software. The material was expanded and revised continuously, with the help of contributors and critics from Britain and abroad. Some areas, notably partial differential equations, were difficult to handle in the library format, but eventually specialised packages became available for these problems, and the library was further enhanced by links to graphical facilities.

Staff appointed at Manchester in the 1970's were Jack Williams in 1971, and Len Freeman in 1976. The special SRC grant for Numerical Analysis supported a number of visitors, including Louis Rall from Wisconsin (1973), Harry Robertson from ICI Runcorn (1973–74) and Charles Van Loan, a postdoctoral fellow who went on to work at Cornell (1974–75). SRC also provided more research studentships, and 22 Ph.D. students began their courses in the years 1970–79. Towards the end of this time the SRC introduced CASE studentships for projects linked to industry, and the Manchester group used these to establish closer collaboration with local firms such as Rolls-Royce and ICI. The number of students on the M.Sc. course increased; a part-time M.Sc. was started in 1973, but the demand was not sufficient to maintain it. Another activity which aimed to disseminate advances in Numerical Analysis was a series of Summer Schools, which were organized jointly by the numerical analysts at Liverpool (under L. M. Delves) and Manchester. The first one, on boundary-value problems, was held at Liverpool in 1971, and succeeding Schools covered integral equations (1973), initial-value problems (1975), partial differential equations (1978), nonlinear problems (1980), and advances in algorithms (1984). The lecturers at these meetings included leading external contributors, and the proceedings of the last five were published by O.U.P. The link with Liverpool also led to cooperation over industrial consultancy and projects; on the Manchester side this work involved mainly Ian Gladwell and Len Freeman.

By the end of the 1970's the position of Numerical Analysis as a branch of Mathematics was well established in undergraduate syllabuses; the number of specialist journals and conferences had increased greatly, and computation was playing a significant role in areas of pure mathematics, as Newman had anticipated in 1948. Computer use became almost universal when powerful desk machines were introduced in the 1980's, and the work which had been done on numerical methods and algorithms provided a good basis for general software packages.

Joan Walsh

5 Report on Workshop "New Frontiers in Computational Mathematics"

A workshop New Frontiers in Computational Mathematics with 63 participants was held over the weekend January 10–11, 2004 at the Chancellors Hotel and Conference Centre, University of Manchester. It was organized by Nick Higham, Tony Shardlow, Françoise Tisseur (University of Manchester) and David Silvester (UMIST) under the auspices of the Manchester Centre for Computational Mathematics, with financial support from the University of Manchester, The London Mathematical Society, the UK and Republic of Ireland SIAM section, the Royal Society and the Wolfson Foundation. The workshop focused on four cutting edge, interdisciplinary research areas of computational mathematics, with each area having a keynote speaker and other contributed talks and posters. Just the briefest highlights are reported here. For more details, see the conference web site (`http://www.maths.man.ac.uk/MCCM/frontiers.html`), which contains links to many of the presentations.

Jack Dongarra (University of Tennessee, Knoxville and Oak Ridge National Laboratory) opened the workshop with a talk "Trends in High Performance Computing and the Grid" in which he discussed the evolution of computational power and how it is measured, and showed how the power is being exploited in diverse computational applications ranging from grid computing to Google. Mikel Lujan (University of Manchester) described how the OoLaLa project is using object technology in the design of high performance linear algebra libraries in order to reduce the number of specialized interfaces, and hence the coding effort, while having minimal impact on performance. Len Freeman (University of Manchester) described a feedback-guided parallel loop scheduling algorithm that was motivated by a collaboration with the UK Meteorological Office.

A diverse session on mathematical biology was opened by Mark Chaplain (University of Dundee), with a fascinating survey of the modelling of cancer cells, and particularly angiogenesis, by describing the evolution of networks of blood vessels. Of interest both for the mathematics and the insight into the workings of our bodies, this session also offered a computational study of airway closure by Andrew Hazel (University of Manchester), (one of the conclusions: keep breathing!), computational models of pattern formation on butterfly wings from Andrew Wathen (Oxford University), and work on the little studied "mathematical modelling of micturation" by urologist C. P. Arun (University College, London). Arun gets the award for the most striking title: "Bladder contraction is rocket science!".

Per Christian Hansen (Technical University of Denmark) lead the session on inverse problems and ill-posed problems, with a talk "Large-Scale Methods for Linear Inverse Problems". Via numerous practical examples, he emphasized the importance of regularization and the advantages of exploiting structure in large-scale problems. Also in this session, Bill Lionheart (UMIST) discussed inverse problems in electromagnetics, including in electrical impedance tomography in medical diagnosis, and described a number of interesting PDE and optimization problems that arise.

The final session on image processing and computer vision was opened by Tony Chan (UCLA), who discussed partial differential equation methods. He treated, among many other things, the "inpainting" problem of filling in an occluded subject in an image—something of interest to all those of us whose thumb tends to get in front of our camera lens without us noticing it until after the picture is taken. Ke Chen (Liverpool) discussed multigrid techniques for solving the PDEs of imaging. Stephen Marsland (University of Manchester), explained the advantages of using diffeomorphisms in image registration, illustrating with the geodesic clamped spline and examples drawn from brain scans.

A notable feature of the meeting was the high standard of the 18 posters, which were professionally produced and very readable.

Overlapping with this meeting was a one and a half day workshop celebrating the 60th birthdays of numerical analysts Jim Varah, Alan George, and Michael Saunders, held at Stanford University, January 9-10, 2004 and organized by Gene Golub (Stanford), Michael Friedlander (Argonne National Laboratory), Chen Greif (University of British Columbia), and Esmond Ng (Lawrence Berkeley National Laboratory). Written greetings from attendees at the New Frontiers meeting were faxed across to Stanford, including best wishes for many more productive years.

In his concluding remarks, David Silvester remarked that this workshop had delimited the frontiers of knowledge in the four areas of computational mathematics considered—an ample result for a weekend's work—and that he hoped that a future more lengthy Manchester workshop would *extend* the boundaries.

Nick Higham

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6 Joint University of Manchester–UMIST Applied Mathematics and Numerical Analysis Seminars

February 5, 2003. Joel Daou (UMIST) Two-dimensional travelling waves and stationary solutions in a reactive counterflow with heat-losses.

March 5, 2003. John Dold, (UMIST) The structure of flames with simple chemical kinetics

March 12, 2003. C. Carstensen (Vienna University of Technology Austria) Mathematical and Computational Aspects of Nonconvex Minimization Problems Allowing for Microstructure

March 19, 2003. Andrew Willmott (Keele) Coastal polynyas; observations and modelling

March 26, 2003. John Mackenzie (Strathclyde) On the solution of moving boundary value problems using adaptive moving meshes.

April 2, 2003 Mark Kelmanson (Leeds) Why weeny water waves weakly wobble, wane and wander whilst whirling

May 7, 2003. John King (Nottingham) Mathematical modelling of quorum sensing and tissue penetration during bacterial infections

May 15, 2003. Jim Denier (Adelaide) Boundary-layer development within the flow in a suddenly blocked channel

May 19, 2003, Avner Friedman (Ohio State) Evolution of free boundaries and their asymptotic behaviour

October 1, 2003. N. Peake (Cambridge) Fluid-structure interactions with mean flow

October 8, 2003. A. McIntosh (Leeds) Burning, Frizzling or Fizzling?

October 22, 2003. M. Roberts (Surrey) Critical point theory for relative periodic orbits of symmetric Lagrangian systems

October 29, 2003. R. P. Behringer (Duke) The Scientist in the Sandbox: Forces and Fluctuations in Granular Materials

November 5, 2003. M. R. Foster (Ohio State) On the evolution of one- and two-sided dendrites

November 12, 2003. C. Sparrow (Warwick) Dynamics and Geometry in an example of Continuous Time Fictitious Play

November 19, 2003. P. Wiberg (Warwick) About parameter estimation for partially observed SDEs

November 26, 2003. J. Barrett (Imperial College) Finite Element Approximation of a Phase Field Model for Electromigration and Stress Voiding.

December 10, 2003. R. S. Johnson (Newcastle) The Camassa-Holm equation for water waves

7 Numerical Analysis Reports

The following reports may be identified by the ISSN number `ISSN 1360-1725` and are available in hard copy (contact The Secretaries, Mathematics Department, University of Manchester, Manchester, M13 9PL, England) and in electronic form via the MCCM web pages at `http://www.ma.man.ac.uk/MCCM/MCCM.html` or `http://www.maths.man.ac.uk/~nareports` to go directly to the reports. Many reports form the basis of papers subsequently published in journals.

The reports are listed in reverse chronological order.

[1] Nicholas J. Higham. The numerical stability of barycentric Lagrange interpolation. Numerical Analysis Report No. 440, Manchester Centre for Computational Mathematics, Manchester, England, December 2003. 10 pp.

[2] Evelyn Buckwar and Tony Shardlow. Weak approximation of stochastic delay differential equations. Numerical Analysis Report No. 439, Manchester Centre for Computational Mathematics, Manchester, England, December 2003.

[3] Tony Shardlow. Nucleation of waves in excitable media by noise. Numerical Analysis Report No. 438, Manchester Centre for Computational Mathematics, Manchester, England, December 2003.

[4] Tony Shardlow. Numerical simulation of stochastic PDEs for excitable media. Numerical Analysis Report No. 437, Manchester Centre for Computational Mathematics, Manchester, England, December 2003.

[5] Philip I. Davies and Nicholas J. Higham. Computing $f(A)b$ for matrix functions f. Numerical Analysis Report No. 436, Manchester Centre for Computational Mathematics, Manchester, England, November 2003. 10 pp.

[6] Judith M. Ford, Neville J. Ford, and John Wheeler. Simulation of grain boundary creep: Analysis of some new numerical techniques. Numerical Analysis Report No. 435, Manchester Centre for Computational Mathematics, Manchester, England, October 2003.

[7] Judith M. Ford and Eugene E. Tyrtyshnikov. Solving linear systems using wavelet compression combined with Kronecker product approximation. Numerical Analysis Report No. 434, Manchester Centre for Computational Mathematics, Manchester, England, October 2003. 11 pp. Submitted to special edition of Numerical Algorithms, Proceedings of Quatrime sminaire sur l'algorithmique numrique applique aux problmes industriels, Calais, 2003.

[8] Rafikul Alam. On the construction of nearest defective matrices to a normal matrix. Numerical Analysis Report No. 433, Manchester Centre for Computational Mathematics, Manchester, England, September 2003. 6 pp.

[9] D. Steven Mackey, Niloufer Mackey, and Françoise Tisseur. Structured factorizations in scalar product spaces. Numerical Analysis Report No. 432, Manchester Centre for Computational Mathematics, Manchester, England, 2003. In preparation.

[10] Christopher T. H. Baker and Eugene I. Parmuzin. Identification of the initial function for delay differential equations: Part i: The continuous problem & an integral equation analysis. Numerical Analysis Report No. 431, Manchester Centre for Computational Mathematics, Manchester, England, January 2004. 25 pp.

[11] Christopher T. H. Baker and Eugene I. Parmuzin. A guided tour of variation of parameters formulae for continuous and discretized DDEs. Numerical Analysis Report No. 430, Manchester Centre for Computational Mathematics, Manchester, England, January 2004. 21 pp.

[12] Manchester Centre for Computational Mathematics. Annual report: January–December 2002. Numerical Analysis Report No. 429, Manchester Centre for Computational Mathematics, Manchester, England, June 2003. 19 pp.

[13] Dario A. Bini, Luca Gemignani, and Françoise Tisseur. The Ehrlich-Aberth method for the nonsymmetric tridiagonal eigenvalue problem. Numerical Analysis Report No. 428, Manchester Centre for Computational Mathematics, Manchester, England, June 2003. 23 pp.

[14] D. Steven Mackey, Niloufer Mackey, and Daniel M. Dunlavy. Structure preserving algorithms for perplectic eigenproblems. Numerical Analysis Report No. 427, Manchester Centre for Computational Mathematics, Manchester, England, May 2003. 30 pp.

[15] Nicholas J. Higham, D. Steven Mackey, Niloufer Mackey, and Françoise Tisseur. Computing the polar decomposition and the matrix sign decomposition in matrix groups. Numerical Analysis Report No. 426, Manchester Centre for Computational Mathematics, Manchester, England, April 2003. 15 pp.

[16] Christopher T. H. Baker, Gennadii A. Bocharov, Christopher A. H. Paul, and Fathalla A. Rihan. Models with delays for cell population dynamics: Identification, selection and analysis. part i: Computational modelling with functional differential equations: Identification, selection, and sensitivity. Numerical Analysis Report No. 425, Manchester Centre for Computational Mathematics, Manchester, England, February 2003. 28 pp.

[17] Nicholas J. Higham, Mihail Konstantinov, Volker Mehrmann, and Petko Petkov. Sensitivity of computational control problems. Numerical Analysis Report No. 424, Manchester Centre for Computational Mathematics, Manchester, England, March 2003. 32 pp.

[18] D. Steven Mackey and Niloufer Mackey. On the determinant of symplectic matrices. Numerical Analysis Report No. 422, Manchester Centre for Computational Mathematics, Manchester, England, February 2003. 12 pp.

[19] D. Steven Mackey, Niloufer Mackey, and Françoise Tisseur. $\mathbb{G}$-reflectors in scalar product spaces. Numerical Analysis Report No. 420, Manchester Centre for Computational Mathematics, Manchester, England, February 2003. 24 pp.

[20] D. Steven Mackey, Niloufer Mackey, and Françoise Tisseur. Structured tools for structured matrices. Numerical Analysis Report No. 419, Manchester Centre for Computational Mathematics, Manchester, England, February 2003. 36 pp.

[21] Judith M. Ford and Eugene E. Tyrtyshnikov. Combining Kronecker product approximation with discrete wavelet transforms to solve dense, function-related linear systems. Numerical Analysis Report No. 418, Manchester Centre for Computational Mathematics, Manchester, England, January 2003.

[22] Christopher T. H. Baker and Christopher A. H. Paul. Piecewise continuous solutions of neutral delay differential equations. Numerical Analysis Report No. 417, Manchester Centre for Computational Mathematics, Manchester, England, December 2003. 35 pp.