



MANCHESTER CENTRE FOR
COMPUTATIONAL MATHEMATICS

Annual Report: January–December 1998

Numerical Analysis Report No. 344

Manchester Centre for Computational Mathematics
Numerical Analysis Reports

DEPARTMENTS OF MATHEMATICS

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A Message from the Director

The Annual Report serves to publicize the work that has taken place during 1998. Along with other MCCM technical reports, information about the M.Sc. in Numerical Analysis and Computing, and MCCM seminar details, it is available from the MCCM Web page at

<http://www.ma.man.ac.uk/MCCM/>

Numerical analysis and computing have a long history at Manchester, and this year saw the celebration of the 50th anniversary of the first computations made in Manchester on the world's first stored program computer. MCCM itself began as a collaborative Centre a number of years ago, to reflect and if possible to strengthen the existing collaboration between the Numerical Analysis Groups at The University of Manchester, at UMIST and with the Mathematics research group at University College Chester, and to provide for Honorary Research Fellows. This collaboration had been manifest in the M.Sc. in Numerical Analysis & Computing, in the seminar programme, and also in the organization of symposia and of mini-symposia at national and international meetings. Research collaboration also reveals itself in a number of jointly-authored papers. Evidence of Collaboration will be found in the following pages.

Numerical Analysis is a broad church and like other sections of Applied Mathematics should be informed by modelling considerations and the practicalities of modern computing, and the subject thrives when there are healthy links with active groups in Mathematics and in Computer Science. These links are seen in Manchester, in particular through the involvements in the Centre for Novel Computing and the celebrations of 50 years of Computing in Manchester, and in collaborative work with applied mathematicians, mathematical biologists, etc. The beginning of 1998 saw interviews for appointments in the Applied Mathematics Group at the University of Manchester, and the appointees have interests that reinforce the broad view of mathematics implicit in such a perspective. Similarly at UMIST, recent appointments in Applied Mathematics have strengthened the general area of Mathematical Modelling. Strong groups in Dynamical Systems and Combustion Theory are being developed in the Department and interaction between these groups and the Numerical Analysis group have started and are expected to grow.

Christopher T. H. Baker
Director of MCCM

Christopher T. H. Baker

Professor of Mathematics

D.Phil., Oxford University, 1964

My three-year term as Head of the Department of Mathematics in the University of Manchester came to a close at the beginning of the academic session 1998-9. Whilst to be Head of Department is an occupation in itself, I found my Department very supportive of me as their Head and I was able to continue my research activity. I consider my main success as Head was my progress in obtaining approval for rejuvenating appointments and for promotions of able staff, since the performance of the whole department in teaching and research depends upon morale.

Up until September 1st., when I was succeeded as Head of Department by Professor Nigel Ray, I had responsibility as Head to ensure that preparations were under way for our "Subject Review" (QAA). (Prof. Nigel Ray undertook to serve as overseer of these preparations but had research leave for the second semester on 1997-8, and Prof. Joan Walsh gave invaluable assistance in these preparations.) The "Subject Review" (in which the Department was awarded a score of 22 out of a possible 24) took place in December 1998. In the event, I had only a limited role in QAA preparations after September 1st.

To a first approximation, my tenure as Head of Department started with RAE 96 and finished at QAA 98.

Since ceasing to serve as Head, I have concentrated upon postgraduate teaching (at present PhD supervision) and research. I have been endeavouring to build up a group working in my current area of interest and centered on the Manchester Centre for Computational Mathematics. At the end of 1998, the group comprises:

University	Chester	UMIST
Prof C Baker	Dr N Ford	Dr R Thomas
Dr C Paul (EPSRC/HEFCE funds)	Dr Liu (visiting)	
Dr Buckwar (EU funds)		
Mr V Wulf (EPSRC from 1/1/99)	Dr Edwards	
Dr Hu (visiting)		
F Rihan (O/S PhD student)	Mr Roberts	
A Filiz (O/S PhD student)	Mr Wulf (to Dec 98)	
H Tian (O/S PhD student)		

I have international contacts involving various levels of cooperation, that most active at present being with Prof Bocharov.

Having been invited to give a plenary talk at Athens I decided to organize a mini-symposium there, and I am now organizing, with Dr Ford, two mini-symposia sessions at ICIAM99 in Edinburgh in 1999 and, with Prof Bellen (Trieste), two mini-symposia sessions in Australia later in 1999.

The above activities have been accomplished with the minimum of HEFCE expenditure, but they do require (apart from the effort of preparing conference papers!) some travel funds and subsistence, where these are not available elsewhere, & occasional computing support. Dr Paul has been funded to work as an RA on an EPSRC grant. My PhD student Hongjiong Tian was funded by an ORS award. On December 1st., Dr Buckwar started her Marie Curie Fellowship to undertake research with me into the numerical solution of stochastic delay differential equations. We are already constructing a further application to follow on from this project.

Appointments and Professional Activities

Member of the EPSRC College (Mathematics Programme)

Head of Department, Department of Pure & Applied Mathematics, for three years to September 1st 1998;

Director, MCCM;

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

Member of Faculty Development Subcommittee, Member of the Dean's Advisory Committee.

Member of the College of the EPSRC Mathematic Programme

Editor, Journal of Computational & Applied Mathematics

Editor, Journal of Integral Equations & Applications

Editor, J Hellenic Math. Soc.

Honorary editor, Communications on Applied Nonlinear Analysis

Member of the accreditation board, Computer Abstracts

Referee for a number of journals and publishers.

Referee for research proposals (Belgium, UK, New Zealand, etc.)

Publications

The following lists my publications (excluding Technical Reports 326, 327, & 335, detailed below in the annual list) published in 1998.

C.T.H. Baker, G.A. Bocharov, C.A.H. Paul & F. Rihan, Modelling and analysis of time-lags in some basic patterns of cell proliferation *Journal of Mathematical Biology*, 37, (1998), no.4, pp.341-371

C.T.H. Baker, & A. Tang, Stability of grazing systems with infinite delays. *Math. Comput. Simulation*, 45 (1998), no. 3-4, pp. 309-317.

C.T.H. Baker, G.A. Bocharov, A. Filiz, N.J. Ford, C.A.H. Paul, F.A. Rihan, A. Tang, R.M. Thomas, H. Tian, D.R. Willé, Numerical modelling by retarded functional differential equations, *Proceedings of the 4th Hellenic European Conference on Computer Mathematics and its Applications*. (editor, E. Lipitakis) pp. 16-39. ISBN 960-85176-7-2.

Lectures

HERCMA-98: Invited plenary talk, Fourth Hellenic Conference on Computer Mathematics & its Applications, Athens, August 1998.

ANODE-98: Invited ("mystery guest") plenary talk at the December 1998 ANODE meeting to mark the retirement of Professor John Butcher, FRSNZ.

Various seminars in the UK

Research Grants

I am currently

- Principal Investigator of EPSRC Research Grant, GR/L35218 on *Numerical strategies for delay and Volterra differential algebraic equations*;
- Scientific supervisor EU TMR Fellowship (Dr E Buckwar) Proposal # ERB4001GT974683 on the topic *Numerical Treatment of Stochastic Functional Differential Equations*;

and have received support from the London Mathematical Society for collaborative research.

Evelyn Buckwar

Marie Curie Research Fellow

Dr. rer. nat. Free University of Berlin, 1997

Appointments and Professional Activities

I arrived in Manchester in December to take up appointment as a Marie Curie Fellow working with Christopher Baker on the EU-funded project “Numerical treatment of Stochastic Functional Differential Equations”

Publications

E. Buckwar & Y. Luchko Invariance of a Partial Differential Equation of Fractional Order under the Lie Group of Scaling Transformations *Journal of Mathematical Analysis & Applications* **227** 1998 pp. 81–97.

J. T. Edwards

Head of Department, University College Chester: Associate member

Ph.D. University of Birmingham, 1972

I am Head of the Department of Mathematics at Chester College and also a founder member of the Chester Applied Mathematics group. I work with Neville Ford and our other co-workers on problems related to the numerical solution of evolutionary problems.

I have recently completed some work relating to the estimation of ranges of parameter values for a Volterra integro-differential equation for which the numerical solution (obtained by a DQ method) exhibits the same qualitative behaviour as the true solution.

Professional Activities

Head of Department of Mathematics, Chester College.

Lectures

Lecture at the IMACS Congress on Computer Simulation and Mathematical Modelling, Alicante, July 1998, (Presented by Jason Roberts) Existence of asymptotically stable solutions for some nonlinear integro-differential equations.

N. J. Ford

Principal Lecturer, University College Chester: Associate member

Ph.D. University of Liverpool, 1991

I continue to work in the field of numerical approximations of solutions of functional differential equations and my particular interest is in establishing conditions under which qualitative behaviour of the true solution is reflected in the numerical approximation. My main collaborator in this work is Christopher Baker, and I also work with John Edwards at Chester. I have worked with three PhD students this year: Volker Wulf is about to submit his thesis on the numerical approximation of solutions to delay differential equations close to a Hopf bifurcation, Jason Roberts continues his work on the qualitative behaviour of solutions to nonlinear integro-differential equations, and Charles Simpson is developing some ideas on the numerical solution of fractional differential equations an area of study which he first encountered while an MSc student working with Luise Blank when she was in Chester.

Jointly with Kai Diethelm (formerly at Hildesheim and now in Braunschweig) I have worked on the problem of solving fractional differential equations when the order of the problem is known only inexactly. This problem arises in certain applications from materials science and can be troublesome when numerical methods are applied. We have developed some initial results which seem to be of some practical application in testing algorithms and reducing the amount of computer time used in calculating approximate solutions.

Professional Activities

Director, Applied Mathematics Research Group, Chester College School of Science and Health, Research Officer, Chester College

Honorary Research Fellow, University of Manchester

Publications

Neville J Ford, Richard H T Edwards and Paul D Crofts Sensitivity of hospital clinic queues to patient non-attendance, Proceedings of the IMACS Congress on Computer Simulation and Mathematical Modelling, Alicante 1998, p243-248

Neville J Ford and Volker Wulf, The use of boundary locus plots in the identification of bifurcation points in numerical approximation of delay differential equations, MCCM Report 322, 1998 pp15

Neville J Ford and Volker Wulf, Numerical Hopf bifurcation for the delay logistic equation, MCCM Report 323, 1998 pp19

Neville J Ford and Volker Wulf, Hopf bifurcation for numerical approximations to the delay logistic equation, Proceedings of the IMACS Congress on Computer Simulation and Mathematical Modelling, Alicante 1998, 249-254

C T H Baker, G A Bocharov, A Filiz, N J Ford, C A H Paul, F A Rihan, A Tang, R M Thomas, H Tian and D R Willé Numerical modelling by retarded functional differential equations, MCCM Report 335, 1998 pp17

Lectures

Seminar at Portsmouth University: Numerical solution of integro-differential equations

Lecture at the second conference on numerical solution of differential equations, Coimbra, February 1998, The use of the boundary locus method in determining Hopf bifurcation points in numerical solution of delay differential equations.

Lecture at the IMACS Congress on Computer Simulation and Mathematical Modelling, Alicante, July 1998, Hopf bifurcation for numerical solution of the delay logistic equation

Featured plenary lecture at the IMACS Congress on Computer Simulation and Mathematical Modelling, Alicante, July 1998, Sensitivity of hospital clinic queues to patient non-attendance

Paper at ICCAM, Leuven, July 1998 (presented by V Wulf, research student) Numerical Hopf bifurcation for a class of delay differential equations.

Paper at HERCMA, Athens, September 1998 (presented by V Wulf, research student) Insight into the qualitative behaviour of numerical solutions to some delay differential equations.

Meeting on Delay Differential Equations, Leuven, December 1998

Visitors

Dr K. Diethelm, University of Hildesheim, Germany, March 1998

Research Grants

I received funding from the University of Hildesheim to visit Dr K. Diethelm for a week in September 1998.

T. L. Freeman

Senior Lecturer in Computer Science & Mathematics

Ph.D. University of Liverpool, 1974

My research interests remain centred on the solution of practical problems in Science and Engineering on high performance computers. This includes development and analysis of numerical algorithms on parallel computers, and the development of numerical libraries and programming tools for parallel computers.

Since July 1997 I have been Director of the Centre for Novel Computing. The centre is an inter-disciplinary group which performs research into techniques, tools and systems that support the exploitation of High Performance Computing (HPC) in the solution of “real applications”; it focuses on Single Address Space Parallel Computers, and has research tracks in applications and algorithms (both numeric and non-numeric), compilation, and run-time/operating systems.

Through the Centre for Novel Computing I am involved directly in three research projects. PINEAPL (Parallel Industrial Numerical Applications and Portable Libraries) is a European-funded project that is developing a numerical software library designed to execute on distributed memory parallel computers. FALSE (Feedback-Guided Affinity Loop Scheduling for Multiprocessors) is a research project funded by EPSRC; the objective is to tackle an important class of load balance problem which arises frequently in scientific applications (particularly in the solution of systems of PDEs), and for which existing load balance techniques perform poorly. Parallel Computation of Matrix Functions is another research project funded by EPSRC; the aim of the project is to develop new algorithms, theory and analysis for parallel computation of some of the matrix functions, such as the logarithm, exponential or sign function, that arise in important application areas.

Appointments

Director, Centre for Novel Computing, Department of Computer Science, University of Manchester.

External Examiner, modular undergraduate degree scheme, Napier University, Edinburgh.

External examiner for Applied Mathematics, University of Wales, Bangor.

External Examiner, M.Sc. degree in Scientific Computing, University of Huddersfield.

Professional Activities

Editor, *Advances in Computational Mathematics*.

Editor, *Parallel and Distributed Computing Practices*.

Technical reviewer for the Information Technologies Programme (Esprit) of the European Commission.

Member of the Organising Committee of the PINEAPL Workshop on “The Use of Parallel Numerical Libraries in Industrial End-user Applications”, Toulouse, France, February, 1998.

Research Grants

Technical contact person for the PINEAPL project (approximately £305,000 at the University of Manchester), funded by the EEC Fourth Framework Workprogramme from January 1996.

Co-investigator (with Professor J. R. Gurd, Department of Computer Science) of the project, “Feedback-guided Affinity Loop Scheduling for Multiprocessors”, (£103,000) funded by the EPSRC from October 1996.

Co-investigator (with Professor N. J. Higham, Department of Mathematics and Professor J. R. Gurd, Department of Computer Science) of the project, *Parallel Computation of Matrix Functions*, (£148,000) funded by the EPSRC from July 1998.

Publications

Bull, J. M. and Freeman, T. L. (1998) *Parallel Algorithms for Multi-dimensional Integration*, Parallel and Distributed Computing Practices, **1**, pp. 25–39.

Ford, R. W., Riley, G. D. and Freeman, T. L. (1998) *The Development of Parallel Optimisation Routines for the NAG Parallel Library*, In **High Performance Algorithms and Software in Nonlinear Optimization**, ed. De Leone, R., Murli, A., Pardalos, P. M. and Toraldo, G., Kluwer Academic Publishers, Dordrecht.

Freeman, T. L., Ford, R. W., Riley, G. D. and Young, P. E. (1998) *Introduction to the PINEAPL and NAG Parallel Libraries*, In Proceedings of PINEAPL Workshop, Toulouse, February 1998, available at <http://www.cerfacs.fr/~touzou/Pineapl/>

Lectures

(with R. W. Ford and G. D. Riley and P. E. Young) *Introduction to the PINEAPL and NAG Parallel Libraries*, PINEAPL Workshop on the Use of Parallel Numerical Libraries in Industrial End-user Applications, CERFACS, Toulouse, France, February 1998.

G. Hall

Senior Lecturer

Ph.D. University of Manchester, 1968

In February I attended the 2nd International Meeting on Numerical Methods for Differential Equations in Coimbra Portugal. I gave a paper at the meeting which has since been accepted for a special issue of the Journal of Computational and Applied Mathematics devoted to the conference.

Mrs Usman was awarded her Ph.D. this year, completing the work on grid selection in Adams codes

Appointments and Professional Activities

External Examiner. School of Computing and Mathematics, Teesside University.

Reviewer for Zentralblatt.

Referee for several journals.

Publications

A.Usman and G.Hall (1998). Equilibrium states for predictor-corrector methods. *Journal of Computational and Applied Mathematics*. **89**. pp. 275–308.

A.Usman and G.Hall (1998). Alternative stepsize strategies for Adams Predictor-corrector codes. *Dept. of Mathematics, University of Manchester, Numer. Anal. Report No. 318*. (Submitted for publication to Journal of Computational & Applied Mathematics).

A.Usman and G.Hall (1998). Modified order and stepsize strategies in Adams codes. *Dept. of Mathematics, University of Manchester, Numer. Anal. Report No. 329*. (Accepted for publication in Journal of Computational & Applied Mathematics).

Nicholas J. Higham

Professor of Applied Mathematics

Ph.D. University of Manchester, 1985

A highlight of the year for MCCM was the meeting “Numerical Analysis and Computers—50 Years of Progress”, held in June 1998 as part of the celebrations to mark the 50th anniversary of the first computations made by the Manchester “Baby”—the world’s first stored program computer. The 90 attendees enjoyed eleven invited talks describing how numerical analysis has been influenced by the development of computers over the last fifty years and predicting future developments; see <http://www.ma.man.ac.uk/NAC98> for reports and photographs, and also the article in the September 1998 issue of SIAM News cited below.

Bobby Cheng successfully defended his thesis in March and subsequently took a postdoctoral position working on the grant *Parallel Computation of Matrix Functions*, held jointly by me, Len Freeman and John Gurd (Department of Computer Science). This grant represents collaboration between the Numerical Analysis Group and the Centre for Novel Computing and good progress has already been made on matrix norm estimation and computation of the matrix logarithm.

SIAM published the second edition of my *Handbook of Writing for the Mathematical Sciences* in September 1998. The first edition (1993) has been adopted as a course text in a number of scientific writing programmes. Based on five further years of writing experience and many comments received I completely revised the book and added new material, including chapters on writing a thesis, giving a talk, and preparing a poster.

Research during the year focused on constrained least squares problems (with Tony Cox, now at Matra Marconi Space UK, Portsmouth), the definite generalized eigenvalue problem (with Bobby Cheng), accurate computation of the singular value decomposition, solution of quadratic matrix equations (with Ph.D. student H.-M. Kim) and generation of test matrices for Jacobi methods for the eigenvalue and singular value problems (with Ph.D. student P. I. Davies).

Appointments

Head of the Numerical Analysis Group.

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

Applied Mathematics/Numerical Analysis seminar organizer.

Professional Activities

Editor, SIAM Journal on Matrix Analysis and Applications.

Associate editor, IMA Journal of Numerical Analysis.

Editor, Linear Algebra and Applications.

SIAM News representative of SIAM Activity Group on Linear Algebra.

Member of Society for Industrial and Applied Mathematics (SIAM) Council.

Member of Executive Committee of Foundations of Computational Mathematics.

Member of Board of Directors of International Linear Algebra Society.

Organizer, with Dr D. J. Silvester and Dr F. Tisseur, of one and a half day meeting “Numerical Analysis and Computers—50 Years of Progress”, University of Manchester, June 1998.

Organizer of minisymposium “Accuracy and Stability in Numerical Linear Algebra”, SIAM Annual Meeting, University of Toronto, July 1998.

Member of Local Organizing Committee of Foundations of Computational Mathematics meeting, Oxford, 1999.

Member of organizing committee of International Linear Algebra Society Conference, Barcelona, 1999.

Member of organizing committee of Householder Symposium XIV, Whistler Mountain, Vancouver, 1999.

Member of Ph.D. thesis defense committee for Fabrice Nativel, *Fiabilité Numérique et Précision Finie: Une Méthode Automatique de Correction Linéaire de l’Erreur d’Arrondi*, Université de la Réunion, Ile de la Réunion (France), December 1998.

Publications

(Most of these publications are available from my Web page at <http://www.ma.man.ac.uk/~higham/>)

N. J. Higham. *Handbook of Writing for the Mathematical Sciences*, Second edition, Society for Industrial and Applied Mathematics, Philadelphia, 1998. xvi+302 pp. ISBN 0-89871-420-6.

S. H. Cheng and N. J. Higham. A modified Cholesky algorithm based on a symmetric indefinite factorization. *SIAM J. Matrix Anal. Appl.*, 19(4):1097–1110, Oct. 1998.

D. J. Higham and N. J. Higham. Structured backward error and condition of generalized eigenvalue problems. *SIAM J. Matrix Anal. Appl.*, 20(2):493–512, 1998.

N. J. Higham and S. H. Cheng. Modifying the inertia of matrices arising in optimization. *Linear Algebra and Appl.*, 275-276:261–279, 1998.

N. J. Higham. Factorizing complex symmetric matrices with positive definite real and imaginary parts. *Math. Comp.*, 67(224):1591–1599, 1998.

A. J. Cox and N. J. Higham. Stability of Householder QR factorization for weighted least squares problems. In D. F. Griffiths, D. J. Higham, and G. A. Watson, editors, *Numerical Analysis 1997, Proceedings of the 17th Dundee Biennial Conference*, volume 380 of *Pitman Research Notes in Mathematics*, pages 57–73. Addison Wesley Longman, Harlow, Essex, UK, 1998.

N. J. Higham. Commentary on Lanczos’s “Introduction” to the “Tables of Chebyshev Polynomials $S_n(x)$ and $C_n(x)$ ”. In W. R. Davis et al., editors, *Cornelius Lanczos Collected Published Papers with Commentaries*, volume VI, pages 3:557–3:559. North Carolina State University, Raleigh, NC 27695-8202, USA, 1998.

A. J. Cox and N. J. Higham. Row-wise backward stable elimination methods for the equality constrained least squares problem. Numerical Analysis Report No. 319, Manchester Centre for Computational Mathematics, Manchester, England, Mar. 1998. To appear in *SIAM J. Matrix Anal. Appl.*

N. J. Higham. Notes on accuracy and stability of algorithms in numerical linear algebra. Numerical Analysis Report No. 333, Manchester Centre for Computational Mathematics, Manchester, England, Aug. 1998. 42 pp. To appear in proceedings of EPSRC Numerical Analysis Summer School, Leicester University, July 1998.

A. J. Cox and N. J. Higham. Backward error bounds for constrained least squares problems. Numerical Analysis Report 321, Manchester Centre for Computational Mathematics, Manchester, England, April 1998, ISSN 1360-1725; to appear in *BIT*.

S. H. Cheng and N. J. Higham. The nearest definite pair for the Hermitian generalized eigenvalue problem. Numerical Analysis Report 325, Manchester Centre for Computational Mathematics, Manchester, England, May 1998, ISSN 1360-1725; to appear in *Linear Algebra and Appl.*

N. J. Higham. QR factorization with complete pivoting and accurate computation of the SVD. Numerical Analysis Report No. 324, Manchester Centre for Computational Mathematics, Manchester, England, September 1998, ISSN 1360-1725; submitted to *Linear Algebra and Appl.*

Contributor (numerical analysis and linear algebra entries) to *The Penguin Dictionary of Mathematics* (David Nelson, editor), Penguin, London, second edition, 1998. ISBN 0-14-051342-6. 461 pp.

N. J. Higham. Review of “Christoph W. Ueberhuber, Numerical Computation: Methods, Software and Analysis, Springer-Verlag, 1997”. *Computational Science and Engineering*, 5(1):79, 1998.

N. J. Higham and D. J. Silvester. “Nothing was Ever the Same Again”. *SIAM News*, 31(7):1,8, September 1998.

Lectures

Seventh Conference of the International Linear Algebra Society, Madison, June 1998. Plenary lecture “QR Factorization with Complete Pivoting and Accurate Computation of the SVD”. Talk in minisymposium “Numerical Linear Algebra”: “The Nearest Definite Pair and the Inner Numerical Radius”.

EPSRC Numerical Analysis Summer School, Leicester University, July 1998. One of three invited lecturers giving five one-hour lectures. Title “Accuracy and Stability of Algorithms in Numerical Linear Algebra”.

International Workshop on Accurate Solution of Eigenvalue Problems, Pennsylvania State University, July 1998. “QR Factorization with Complete Pivoting and Accurate Computation of the SVD”.

“Can You ‘Count’ on Your Computer?”, Public lecture in Science Week, University of Manchester, March 1998.

SIAM Annual Meeting, University of Toronto, July 1998. Talk in minisymposium “Accuracy and Stability in Numerical Linear Algebra”: “Householder QR Factorization with Complete Pivoting: Why and When to Use It”.

Seminar at Université de la Réunion (France).

Research Grants

Principal investigator on project “Numerical Analysis of the Generalized Eigenvalue Problem” funded by EPSRC Mathematics Committee for three years from January 1998 (value £117,284). Grant GR/L76532. Provides a postdoctoral research assistant, travel and computer equipment.

Principal investigator on project “Parallel Computation of Matrix Functions” funded by 50% by EPSRC Systems Architecture Committee and 50% by DERA, Malvern for three years from October 1998 (value £156,157). Co-investigators Dr T. L. Freeman and Professor J. R. Gurd. Grant GR/L94314. Provides a postdoctoral research assistant, travel and computer equipment.

Co-investigator with Professor A. I. Ruban on project “Advanced Numerical Methods to Calculate 3D Flow Separation” funded by EPSRC Mathematics Committee for three years from October 1998 (value £114,630). Grant GR/L62580. Provides postdoctoral research assistant, travel and computer equipment.

Co-investigator with Professor A. I. Ruban on project “Advanced Numerical Methods to Calculate 3D Flow Separation” providing an EPSRC Visiting Fellowship for Professor J. D. A. Walker for three years from May 1998 (value £3,000). Grant GR/M02828.

Christopher A. H. Paul

Temporary Lecturer/Research Associate
Ph.D. University of Manchester, 1992

My research throughout this year has been associated with Christopher Baker’s EPSRC grant on *numerical strategies for delay and Volterra differential algebraic equations*; initially being employed on the grant as the Research Associate, and subsequently being employed by the University as an Experimental Officer. During the latter period, the demands on my time from my computer support officer role severely reduced my research activity. However, despite this, I was still able to attend the HERMCA 98 conference in Athens during August.

Appointments and Professional Activities

Computer Support Officer, Department of Mathematics

Publications

C.T.H. Baker, G.A. Bocharov, C.A.H. Paul, F.A. Rihan, Modelling and analysis of time-lags in some basic patterns of cell proliferation, *Journal of Mathematical Biology*, 37, 1998 (4), pp. 341-371.

C.A.H. Paul, The treatment of derivative discontinuities in differential equations, Proceedings of 4th Hellenic European Conference on Computer Mathematics and its Applications.

C.A.H. Paul, An introduction to the Mathematics Department Unix system, Computer Support documentation.

C.A.H. Paul, A guide to the Mathematics Department ground floor PC cluster, Computer Support documentation.

C.T.H. Baker, G.A. Bocharov, A. Filiz, N.J. Ford, C.A.H. Paul, F.A. Rihan, A. Tang, R.M. Thomas, H. Tian, D.R. Willé, Numerical modelling by retarded functional differential equations, *Proceedings of 4th Hellenic European Conference on Computer Mathematics and its Applications*.

Lectures

HERMCA 98: Invited mini-symposium talk, Athens, August 1998.

David J. Silvester

Senior Lecturer

Ph.D. University of Manchester, 1984

My main research effort over the year was directed towards the study of a posteriori error estimators, and developing adaptive refinement strategies for solving the (steady-state) Navier-Stokes equations governing viscous incompressible flow. This project has a powerful engine-room which is manned by a research assistant, David Kay, and a Ph.D student, Sean Norburn. Two papers outlining our progress have been published to date, and another two are currently in preparation. David moved to the Oxford University Computing Laboratory over the summer. He is now working on the development of fast iterative solvers as part of ongoing collaboration with Andy Wathen.

At the end of June, I joined forces with Allan Barker to give a ten day summer school on “Iterative and finite element multigrid methods” at the Technical University of Denmark. The practical sessions were organised around some user-friendly matlab software which was written by myself and Howard Elman from the University of Maryland, USA. This software can be used to generate typical matrix systems which arise when using finite element approximation methods to solve test problems which arise in fluid dynamics; specifically, convection-diffusion problems, and driven cavity flows governed by the Stokes and Oseen equations. The latest release (version 1.3) of the software includes a number of multigrid convection-diffusion solvers which can be explored by the interested user. (The software is freely available from <http://www.ma.umist.ac.uk/djs/>).

Research Grants

Principal Investigator on project “Numerical Analysis of Convection-Diffusion Problems”, NATO collaborative grant CRG 960782, October 1996–September 1998 (value £3500).

Principal Investigator on project “Analysis of Numerical Methods for Incompressible Fluid Dynamics”, EPSRC grant GR/K91262, October 1996–September 1999 (value £89,000, funds a PDRA for 18 months and a three year Ph.D studentship).

Publications

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

Fischer, B., Ramage, A., Silvester, D. and Wathen, A. Minimum residual methods for augmented systems, *BIT*, 38, pp. 527–543, 1998.

Norburn, S. and Silvester, D. Stable vs. stabilised mixed methods for incompressible flow, *Computer Methods in Applied Mechanics and Engineering*, 166, pp. 131–141, 1998.

Silvester, D. Stabilised mixed finite element methods., in *Incompressible Flow and the Finite Element Method*, Gresho P. and Sani R., Wiley, New York, pp. 533–549, 1998.

Wathen, A., Fischer, B. and Silvester, D. The convergence of iterative solution methods for symmetric and indefinite systems. *Numerical Analysis 1997*, Griffiths D., Higham D. and Watson G. (Eds), Longman Scientific, pp. 230–240, 1998.

Lectures

“Multigrid preconditioning in computational fluid dynamics,”
Manchester Metropolitan University, January 1998.

“A posteriori error estimation for elliptic PDEs,”
University of Strathclyde, February 1998.

Invited speaker at a *Summer School on Iterative and Finite Element Multigrid Methods*, held at the Technical University of Denmark, June 1998.

“A posteriori error estimation for elliptic PDEs,”
Imperial College, December 1998.

R. W. Thatcher

Senior Lecturer

Ph.D. University of London, 1972

Being head of a major Mathematics Department makes great demands on my time and the amount of effort I am able to devote to my own research is inevitably limited. I see a major part of my input into research at UMIST as creating the atmosphere and environment for staff in the Department to do their own research at a time when university funds are very limited. Nevertheless, I have some time for my own research and I am working in two main areas. I have a PhD student, Paul Bolton, working on least squares methods for Stokes and Navier Stokes equations; developing a new method for implementing least squares for such problems. My main research activity, however, has been working on Numerical Modelling in Combustion in collaboration with John Dold, also at UMIST. The former area of research is more traditional Numerical Analysis, analysing the quality and effectiveness of the method and comparing it with other methods. On the other hand, the latter area is much more in the area of Computational Physics; using the results of computational models to get an insight into the physical behaviour of flames.

Appointments and Professional Activities

Head of the Mathematics Department, UMIST.

External Examiner for PhDs at Aberystwyth University and Nottingham Trent University.

Publications

On the Least-Squares Method for the Biharmonic Equation. MCCM Report 330.

Ruth M. Thomas

Senior Lecturer

Ph.D. University of Manchester, 1979

In 1998, I worked on six main research projects. The first project involves an investigation of numerical strategies for delay and Volterra differential algebraic equations. This is joint work with Professor Christopher Baker and our Postdoctoral Research Assistant, Dr. Christopher Paul. Our work is supported by a Research Grant from the EPSRC.

The second project concerns the numerical solution of periodic initial value problems with oscillatory solution. Together with my Ph.D. student Monish Luthra, I worked on deriving efficient numerical methods and developing the associated computer software for solving such problems. Monish submitted his Ph.D. thesis in December 1998. Another of my Ph.D. students, Muhammad Gul, is working on developing efficient predictors and interpolants for use with a family of hybrid methods for solving second order initial value problems in ordinary differential equations.

A third project on which I worked concerns the numerical solution of Schrödinger's equation. Here, I collaborated with Dr. Theodore Simos of the University of Thrace on deriving and analysing the properties of a family of exponentially-fitted methods.

In the fourth 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 Thebe Basebi, a Ph.D. student.

During the year, I also worked on symplectic integrators for Hamiltonian problems with a M.Sc. student, Anastasios Papadopoulos, and on continuation methods for solving differential algebraic boundary value problems, in collaboration with a research student, Novia Nasiruddin.

Appointments and Professional Activities

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

R. M. Thomas and T. E. Simos. A family of hybrid exponentially fitted predictor-corrector methods for the numerical integration of the radial Schrödinger equation. *Journal of Computational and Applied Mathematics*, **87**, 215-226 (1997).

C. T. H. Baker, G. A. Bochorov, A. Filiz, N. J. Ford, C. A. H. Paul, F. A. Rihan, A. Tang, R. M. Thomas, H. Tian and D. R. Willé. Numerical Modelling by Retarded Functional Differential Equations. *Numerical Analysis Report No. 335, Manchester Centre for Computational Mathematics, October 1998*. (To appear in the Proceedings of the Athens Conference on Computer Mathematics.)

Research Grants

Co-investigator (with Professor Christopher Baker) on project *Numerical Strategies for Delay and Volterra Differential Algebraic Equations*, EPSRC Grant GR/L35218, June 1997-May 1999 (value £71703).

Lectures

In April 1998, I gave an invited seminar at Manchester Metropolitan University entitled *Shooting and Global Techniques for Differential Algebraic Boundary Value Problems Arising in Detonation Modelling*.

Visitors

Dr. Xiang Kai Li, from Southwest Petroleum Institute, Nanchong, Sichuan, P. R. China, visited me from March to September 1998.

Françoise Tisseur

Research Associate

Ph.D. University of St. Etienne, 1997

My research interests are in numerical linear algebra, focusing particularly on eigenvalue problems and their parallelization.

During my year in the U.S. in 1997 I worked with Professor Jack Dongarra on the LAPACK and ScaLAPACK projects. LAPACK is a linear algebra library of Fortran software and ScaLAPACK is its parallel version for distributed memory architectures. I worked on a parallel divide and conquer code that will be incorporated in the next release of ScaLAPACK. This work has been written up and has been accepted for publication in *SIAM J. on Scientific Computing*.

Since January 1998, I have been working at the University of Manchester as research associate on an EPSRC grant. My current research concerns polynomial eigenvalue problems (generalized and quadratic) and statistical matrix p -norm estimation.

Polynomial eigenvalue problems appear often in the dynamic analysis of structural systems and have many industrial applications, such as the analysis of automobile brakes. I am in contact with Dr L. Komzsik from The MacNeal-Schwendler

Corporation, the producers of the NASTRAN finite element software package, whose users need to solve such problems. My aim is to further our understanding of the quality of the computed solutions. I am developing new methods to test the accuracy of the computed solutions via computable condition numbers and backward errors and I am looking at iterative refinement of the solutions.

A common task in evaluating condition numbers and error bounds is to estimate the norm of a matrix A given implicitly as an operator where only matrix-vector products Ax and $A^T x$ are possible, as is the case in the automobile brake application. I have been looking at the approximation of $\|A\|$ by sampling $\|Ax\|/\|x\|$ at a vector x from an appropriate statistical distribution and at the probability that the estimate is within a certain factor of the true norm in order to provide a level of confidence that a good estimate will be obtained. I am also looking, with Nick Higham, at extending the 1-norm power method to block form. One application is to computation of 1-norm pseudospectra.

Publications

F. Tisseur and J.J. Dongarra. Parallelizing the Divide and Conquer Algorithm for the Symmetric Tridiagonal Eigenvalue Problem on Distributed Memory Architectures. Numerical Analysis Report No. 319, Manchester Centre for Computational Mathematics, Manchester, England, Mar. 1998. (Also Technical Report CS-1998-381, University of Tennessee, March 1998, LAPACK Working Note 132.)

F. Tisseur. Backward Error and Condition of Polynomial Eigenvalue Problems, Numerical Analysis Report 332, Manchester Centre for Computational Mathematics, September 1998. To appear in *Linear Algebra and its Applications*.

F. Tisseur and J. J. Dongarra. A Parallel Divide and Conquer Algorithm for the Symmetric Eigenvalue Problem on Distributed Memory Architectures. To appear in *SIAM J. on Scientific Computing*.

Lectures

Seventh Conference of the International Linear Algebra Society, Madison, June 1998. "Backward Error and Condition Numbers of the Quadratic Eigenvalue Problem".

Invited lecture at EPSRC Numerical Analysis Summer School, Leicester University, July 1998, "The Quadratic Eigenvalue Problem: Backward Error and Condition".

SIAM Annual Meeting, University of Toronto, July 1998. "Parallel Divide and Conquer Algorithm for the Hermitian Eigenvalue Problem".

International Workshop on Accurate Solution of Eigenvalue Problems, Pennsylvania State University, July 1998. "Backward Error and Condition Numbers of Polynomial Eigenvalue Problem".

Seminar at University of Manchester, England, October 1998, "Backward Error and Condition of Polynomial eigenvalue Problems".

Seminar at Université de la Réunion, Department of Mathematics, Ile de la Réunion, France, December 1998.

Professional Activities

Co-organizer, with N. J. Higham and D. J. Silvester, of one and a half day meeting “Numerical Analysis and Computers—50 Years of Progress”, University of Manchester, June 1998.

Joan E. Walsh

Emeritus Professor

D.Phil., Oxford University, 1961

My present research interests are in variational methods for boundary-value equations and elliptic equations, and methods for obtaining limits on the solution using monotonicity. Applications include time-dependent diffusion processes, and nonlinear equations arising in mathematical biology.

Professional Activities

External examiner for B.Sc., Imperial College.

Jack Williams

Senior Lecturer

D.Phil. University of Oxford, 1968

My main research interests continue to be in the the numerical solution of stiff ordinary differential with special interest in aspects of the BDF and implicit Runge–Kutta methods. My two Ph.D. students are now working in these areas. Also I am also collaborating with J. A. King–Hele on the numerical solution of a class of elliptic partial differential equations which arise in the modelling of gas flow circulation in detonation delay elements. The problems include a mixed boundary condition and a pure Neumann condition.

Publications

Ronald Tshelametse and Jack Williams. A new termination criterion for nonlinear iterations in ODE codes. Numerical Analysis Report No. 334, Manchester Centre for Computational Mathematics, Manchester, England, October 1998. 23 pp.

Short-Term Visitors

Professor Gennadii Bocharov, Russian Academy of Sciences, Moscow;

Dr K. Diethelm, University of Hildesheim, Germany;

Dr Guang Da Hu, Japan;

Dr. Xiang Kai Li, Southwest Petroleum Institute, Nanchong, Sichuan.

Numerical Analysis Seminars

The numerical analysis seminars are now largely integrated as part of the joint Manchester-UMIST Applied Mathematics seminars. However, a special afternoon programme of Numerical Analysis Seminars was organised for

October 7, 1998:

2.30pm Dr. Ron Thatcher (Dept. of Mathematics, UMIST) Least Squares, Finite Element Solution of Differential Equations .

3.45 pm Dr. Francoise Tisseur (Dept. of Mathematics , Univ. of Manchester) Backward Error and Condition of Polynomial Eigenvalue Problems .

4.30 pm Prof. Nick Higham (Dept. of Mathematics , Univ. of Manchester) Computing the Singular Value Decomposition to High Relative Accuracy

Numerical Analysis Reports

Most of these reports are available from the MCCM Web page with URL <http://www.ma.man.ac.uk/MCCM/MCCM.html>, and by anonymous ftp from [ftp.ma.man.ac.uk](ftp://ma.man.ac.uk/pub/narep) in `pub/narep` (see the README file therein).

- 317 F. Tisseur and J. Dongarra
Parallelizing the Divide and Conquer Algorithm for the Symmetric Tridiagonal Eigenvalue Problem on Distributed Memory Architectures
March 1998
- 318 Anila Usman and George Hall
Alternative Stepsize Strategies for Adams Predictor-Corrector Codes
February 1998
- 319 A. J. Cox and N. J. Higham
Row-Wise Backward Stable Elimination Methods for the Equality Constrained Least Squares Problem
March 1998
- 320 MCCM
Annual Report 1997
March 1998
- 321 A. J. Cox and N. J. Higham
Backward Error Bounds for Constrained Least Squares Problems
April 1998
- 322 N. J. Ford and V. Wulf
The use of boundary locus point plots in the identification of bifurcation points in numerical approximation of delay differential equations
March 1998
- 323 N. J. Ford and V. Wulf
Numerical Hopf bifurcation for the delay logistic equations
March 1998
- 324 N. J. Higham
QR Factorization with Complete Pivoting and Accurate Computation of the SVD
September 1998

- 325 S. H. Cheng and N. J. Higham The Nearest Definite Pair for the Hermitian Generalized Eigenvalue Problem May 1998
- 326 C. T. H. Baker and A. Tang
Stability of continuous Theta-methods for nonlinear delay differential equations
May 1998
- 327 C. T. H. Baker and A. Tang
Stability of Non-linear Delay Integro-differential Equations via Approximating Equations
May 1998
- 328 A. F. McDonald and J. Walsh
Numerical studies of the FitzHugh-Nagumo equations
June 1998
- 329 A. Usman and G. Hall
Modified Order and Step-size Strategies in Adams Codes
July 1998
- 330 R. Thatcher
On the least-squares method for the biharmonic equation
August 1998
- 331 J. L. Barlow
More Accurate Bidiagonal Reduction for Computing the Singular Value Decomposition
August 1998
- 332 F. Tisseur
Backward Error and Condition of Polynomial Eigenvalue Problems
August 1998
- 333 N. J. Higham
Notes on Accuracy and Stability of Algorithms in Numerical Linear Algebra
August 1998
- 334 R. Tshelametse and J. Williams
A New Termination Criterion for Nonlinear Iterations in ODE Codes
October 1998
- 335 C. T. H. Baker, G.A. Bocharov, A. Filiz, N.J. Ford, C.A.H. Paul, F.A. Rihan, A. Tang, R.M. Thomas, H. Tian D.R. Willé
Numerical Modelling by Delay & Volterra Functional Differential Equations

Continued ...

Postgraduates in Numerical Analysis and Computing 1997-8

M.Sc. by Method I (organized jointly by The University and UMIST)

(Students were registered at the University unless indicated.)

Name	support	first degree	Institution	Comment
Crudge, Sarah E.	EPSRC	B.Sc.	Manchester	
Fazil, Abeda	EPSRC	B.Sc.	Manchester	
Horrocks, Robert	EPSRC	B.Sc.	Dundee	
Nasuhioglu, Sedef		B.Sc.	Turkey	
Roy, Kevin	EPSRC	B.Sc.	Manchester	
Thomson, Paula	EPSRC	B.Sc.	Dundee	
Dafik	Scholarship	B.Sc.	Indonesia	(UMIST Registered)
Anastasios Papadopoulos	self	B.Sc.	UMIST	(UMIST Registered)
Katherine Tomlinson	EPSRC	B.Sc.	Nottingham	(UMIST Registered)

Students reading for the degree of PhD

PhD students registered at The University

Ph.D. Year 1

Name	support	first degree	Institution	PhD Supervisor
Davies, Philip I.	EPSRC Case	B.Sc.	Manchester	N.J. Higham
Kim, Hyun Min	Self-supp	B.Sc.	Korea	N.J. Higham
Tian, Hongjiong	ORS/Dept	B.S.	Shanghai	C.T.H. Baker

Ph.D. Year 2

Name	support	first degree	Institution	PhD Supervisor
Filiz, Ali	Turkey	B.Sc.	Turkey	C.T.H. Baker
Rihan, Fathalla	Egypt	B.Sc.	Egypt	C.T.H. Baker
Tshelametse, Ronald	Scholarship	B.Sc.	Botswana	J. Williams

Ph.D. Year 3

Name	support	first degree	Institution	PhD Supervisor
Al-harbi, Saleh	S. Arabia	B.Sc.	S. Arabia	J. Williams

Ph.D. Writing-up

Name	support	first degree	Institution	PhD Supervisor
Cheng, Sheung Hun	ORS/Self	B.Sc.	Manchester	N.J. Higham
Cox, Anthony	EPSRC	B.Sc.	Manchester	N.J. Higham
Usman, Anila	Pakistan	B.Sc.	Pakistan	G. Hall

PhD students registered at UMIST

Year 1

Name	support	first degree	Institution	PhD Supervisor
Thebe Basebi	Scholarship	BSc	Botswana	R.M. Thomas
Syamsudhuha	Scholarship	BSc	Indonesia	D.J. Silvester
Paul Bolton	EPSRC	BSc	UMIST	R.W. Thatcher

Year 2

Name	support	first degree	Institution	PhD Supervisor
Sean Norburn	EPSRC Project	BSc	UMIST	D.J. Silvester
Muhammad Gul	Pakistan Scholarship	BSc	Pakistan	R.M. Thomas

Year 3 and higher

Name	support	first degree	Institution	PhD Supervisor
Novia Nasiruddin	Scholarship	BSc	Malaysia	R.M. Thomas
Monish Luthra	self	MSc	London	R.M. Thomas

PhD students registered at Chester

Ph.D. Year 2

Name	support	first degree	Institution	PhD Supervisor
Wulf, Volker	Bursary	Diplom.	Rostock	Dr N.J. Ford

Ph.D. Year 3 (Part Time)

Name	support	first degree	Institution	PhD Supervisor
Roberts, Jason	Employer	B.Sc.	Liverpool	Dr N.J. Ford

MSc students registered at Chester College

The MSc course at Chester College can be taken part-time; this list indicates those completing the course this year.

Finishing MSc students

Name	support	first degree	University	Comment
Davies, Neil	Self	B.Sc.	Open	
Hiller, Bryan	Sponsored	B.A.	Liverpool	
Killen, Paul	Self	B.Ed.	Lancaster	
Lee, Rebecca	Snowdon Found.	B.Sc.	Hull	
Little, A. John	ESF	B.Sc.	Liverpool	
Owens, Robert	ESF	B.Sc.	Liverpool	