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UNIVERSITY OF MANCHESTER

Manchester Centre for
Computational Mathematics

$\mathcal{MCCM}$

Annual Report 1992

June 9, 1993

Message from the Director

The History of Numerical Analysis at Manchester

Numerical analysis has for long been a subject of interest at Manchester. The formation of a numerical analysis group in the Department of Mathematics at the University of Manchester dates back to the mid-1960's and the organisational initiative of Joan Walsh, who strengthened the role of numerical analysis. At a similar time in the Department of Mathematics in the Faculty of Technology (UMIST), computational mathematics was made a major element of the undergraduate degree programme under the guidance of R. Butler. Cornelius Lanczos visited UMIST several times in a five year period around 1970 presenting a number of lectures, some of which were recorded. These films are being used at the conference to celebrate the centenary of his birth at North Carolina State University in December 1993.

The Diploma/M.Sc. course was conducted for many years as a cooperative effort between the Department of Mathematics and the Department of Computer Science in the Faculty of Science, and there was a public face in a series of "state-of-the-art' summer schools (conducted jointly with computational scientists at Liverpool University) and a continuing education training (CET) series. External research collaboration with industry and with the Numerical Algorithms Group (NAG Ltd.) has been, and continues to be, a feature of numerical analysis at Manchester, as are research links with industrial researchers and academic staff in other institutions and other countries.

The two groups of Manchester numerical analysts, in the Departments of Mathematics of the University and UMIST, collaborate on the production of technical reports, in conducting an active seminar programme, and in hosting visitors, as well as other areas now linked by tradition to the Manchester numerical analysts. In addition to the numerical analysts, the applied mathematicians count amongst their number many whose research involves computational techniques and some who have an interest in parallel numerical algorithms.

Creation of MCCM

The strengthening of already active groups in computational mathematics and numerical analysis, and the cooperative efforts taking place, made the creation of the *Manchester Centre for Computational Mathematics* a natural step. The numerical analysts at UMIST have for some time played a recognised role in providing lectures and supervision in the M.Sc. in Numerical Analysis and Computing, along with their colleagues in the Mathematics Department and in the Computer Science Department, and this has recently been made a joint M.Sc. between the two institutions. There has also been a move to maintain an expanded Ph.D. program. The creation of MCCM received approval from the University and from UMIST during 1992.

The research interests in parallel numerical analysis have received added impetus through links with the Centre for Novel Computing (CNC), which is located in the Computer Science Department. The CNC houses a Kendall Square Research KSR1 virtual shared memory MIMD computer. Most members of the MCCM are affiliated to CNC and the groups collaborate in European community-funded projects[1], organisation

[1]Notably the APPARC project. The CNC produces its own annual report, to which readers are

of symposia, etc. The CNC places great emphasis on areas of practical interest in parallel computing, and the interests of the numerical analysts (whilst drawing from many areas of mathematics for the theoretical foundations) are also driven in part by modelling of practical problems.

The high research standing of mathematics at Manchester was given recognition when the UFC Research Assessment Exercise (applied throughout the UK) awarded the Applied Mathematics unit of assessment (which includes numerical analysis) a Grade 5, that at UMIST attaining a Grade 4. These high grades were supported by high grades awarded to the other mathematics units (Pure Mathematic, Statistics and Operations Research), and a Grade 5 for the Computer Science Department.

The research papers of the numerical analysts in MCCM are published through the normal academic journals, but to hasten dissemination many are preprinted as NA technical reports that are distributed worldwide to libraries and individual research workers. Details of reports published in 1992 appear below.

Starting in May 1993, most future NA reports will be available by anonymous ftp from `vtx.ma.man.ac.uk (130.88.16.2)` in `pub/nareps` (see the `README` file therein).

Membership of MCCM

Holders of full-time appointments in numerical analysis at Manchester University and at UMIST are automatically members of MCCM, and holders of temporary or visiting appointments and research assistants are temporary members during the tenure of their appointment. The boundaries between numerical analysis and computational applied mathematics are not well-defined and computational applied mathematicians in the two institutes are regarded as associated members of MCCM where their activities make this appropriate. Provision will also be made at some future date for a limited number of numerical analysts in neighbouring institutions, who have links with the group, and other numerical analysts with former or continuing links, to be invited to assume affiliate membership of MCCM.

In the following, we report on the work of the members of MCCM during 1992.

Christopher T. H. Baker, May 1993

referred.

Christopher T. H. Baker

Professor of Mathematics
D.Phil., Oxford University, 1961

My academic activities during the calendar year were heavily influenced by two external commitments. The first of these was my role as convenor of the LMS and SERC-supported Durham Symposium on the theory and numerical analysis of evolutionary problems, which was held between the 4th and 14th July 1992 and was attended by 90 mathematicians from many different nations. The administrative burden associated with this event was shared by Dr Ruth Thomas (UMIST) and we were very grateful for advice from an able UK-based committee and assistance from Durham University. I wish to take this opportunity to thank Dr Thomas for her invaluable contribution. The meeting involved an intensive programme of academic activity from breakfast to evening. Abstracts of the presentations are given in a technical report (No 214). It was approximately a decade ago that I convened my first Durham Symposium, the earlier one being on the numerical treatment of integral equations, and the role of integral equations in applied mathematics; it takes about ten years to forget the effort involved, but the appreciative comments of participants are a reward! A number of the participants at the Durham symposium spent some time in Manchester prior to the meeting and were able to continue or initiate research collaboration; these included Professor John Butcher (adapting STRIDE for delay equations), Professor Kevin Burrage (parallel computing) Professor Vladimir Kolmanovskii (modelling of chemostat systems).

The second commitment was as a member of the Mathematics Assessment Panel in the UFC Research Assessment Exercise. Having had joint responsibility for submitting our departmental report on research activity in the applied unit of research, the autumn of 1992 found me devoting about 21 man-days of time to the task of assessing approximately 65 "units of research" in applied mathematics in universities and other institutes of higher education around the UK. The uplifting aspect of this undertaking was the impression that I gained of buoyant and high quality research activity in applied mathematics and numerical analysis around the UK. Nevertheless, it came as a relief to depart in December for a period as a guest of Professor Butcher at the University of Auckland.

These external commitments, and the annual representations on behalf of members of staff and departmental computing needs have been leavened by continued research activity. In November, my former Ph.D. student Christopher Paul assumed a position as my Research Assistant and we continue to work on delay differential equations. Arsalang Tang works with me on the analysis and numerical modelling of Volterra functional equations and the chemostat equation, and links with former doctoral students [Dr David Willé (Heidelberg), Dr Neville Ford (Chester College) and Dr Mishi Derakhshan (NAG, Oxford)] are maintained. The emphasis is on stability, qualitative behaviour, robust algorithms, and parallel methods. I have recently undertaken some work in nonlinear numerics for differential equations, and hope to apply it to parallel numerical methods. I continue an interest in the numerical solution of integral equations but my present research interest is mainly in the area of evolutionary problems, such as Volterra equations.

Appointments and Responsibilities

Director, Manchester Centre for Computational Mathematics

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

Appointed adjudicator, Fox Prize in Numerical Analysis. Member, Scientific Committee, International Conference on Computational and Applied Mathematics.

Member of the LMS Durham Symposia Committee, 1992–.

External Examiner, M.Sc. degree, University of Reading

University responsibilities include the following: Deputy to the Head of Department, Head of the Numerical Analysis Group (University of Manchester); Member of the Dean's Advisory Committee, and of the Teaching Standards Committee, Faculty of Science; Member of the University Research Support Subcommittee.

Professional Activities

Editor for IMA J. Numerical Analysis

Editor for J. Computational & Applied Mathematics

Editor for J. Integral Equations & their Applications

Editor for Advances in Computational Mathematics

Referee for numerous papers and research proposals.

Publications

(with D.R. Willé) *The tracking of derivative discontinuities in systems of delay-differential equations* Applied Numerical Mathematics, **9** pp. 209–222 (1992)

(with N.J. Ford) *Stability properties for the approximate solution of a delay–integro–differential equation* Applied Numerical Mathematics **9** pp. 357–370 (1992)

(with D.R. Willé) *DELSOL– a numerical code for the solution of systems of delay-differential equations* Applied Numerical Mathematics, **9** pp. 223–234 (1992)

C.T.H. Baker, J.C. Butcher and C.A.H. Paul, Experience of STRIDE applied to delay differential equations, Numerical Analysis Report No. 208, University of Manchester, January 1992.

C.T.H. Baker and C.A.H. Paul, Explicit Runge–Kutta methods for the numerical solution of singular delay-differential equations, Numerical Analysis Report No. 212, University of Manchester, April 1992.

C.T.H. Baker, Stability functions for multistep formulae for Volterra functional equations, Numerical Analysis Report No. 220, University of Manchester, October 1992.

Lectures

Presented a seminar at the Mathematics Department, Durham University, March 1992.

Presented a lecture at the LMS symposium on evolutionary problems, July 1992, on the effect of nonlinearity and delay in evolutionary problems.

Presented a seminar at the Mathematics Department, University of Manchester, October 1992, on the dynamics of the discretized logistic equation and delayed logistic equation.

Research Grants

SERC Research Grant (approx. £55,000) on *Numerical Analysis and Parameter Estimation for Functional Differential Equations* for two years commencing November 1992.

(With Professor Scholl of Durham University): Investigator; Convenor, SERC-funded *LMS Durham Symposium on Evolutionary problems*, 4th–14th July 1992 (£29,720).

Royal Society New Zealand travel grant for partial support of a visit to Professor Butcher, University of Auckland, December 1992–January 1993.

Investigator in collaborative grant funded by ESPRIT Basic Research Action Programme, titled "Performance-critical Applications of Parallel Architectures" (APPARC). Involves nine European institutions. Manchester group headed by Prof. J. Gurd, Computer Science; approximately £157,000 over three years, starting April 1992.

Christian C. Beardah

Temporary Lecturer
Ph.D., University of Manchester Institute of Science and Technology, 1992

In February of 1992 I completed my doctoral oral examination and subsequently received the degree of Ph.D. later in the year. (The thesis, entitled *Finite Difference Solution of Differential/Algebraic Boundary Value Problems Arising in the Modelling of Unconfined Detonations* was submitted in October 1991.)

Throughout the year I continued my research into systems of Differential/Algebraic Equations, in particular those posed as Boundary Value Problems. This research has been in collaboration with my former Ph.D. supervisor, Dr R. M. Thomas (UMIST) and with ICI plc. (See Dr Thomas' entry for more details.) In addition, I have recently been investigating a family of eigenproblems arising in an application of Theoretical Physics. This work is jointly with Professor G. Woolley of The Nottingham Trent University, where I am now situated.

Publications

C. C. Beardah and R. M. Thomas. Two mathematical models of unconfined detonation and their numerical solution. To appear in: *Circuits, Systems and Signal Processing*

Lectures

"The Numerical Solution of Differential-Algebraic Boundary Value Problems Arising in Detonation Theory." SIAM 40th Anniversary meeting, Los Angeles, California, U.S.A..

Research Grants

Royal Society travel grant of £450 enabling travel to the above conference.

T. L. Freeman

Senior Lecturer elect
Ph.D. University of Liverpool, 1974

During the year I continued my work on the development of numerical algorithms suitable for implementation on parallel computers.

In May my textbook *Parallel Numerical Algorithms* was published in the Prentice Hall International Series in Computer Science. The book is jointly authored with Dr. C. Phillips of the University of Newcastle-upon-Tyne and investigates parallel algorithms for a wide range of numerical problems (linear algebra, quadrature, non-linear equations, optimisation, and ordinary and partial differential equations. The book also includes material on the hardware and software (programming languages) aspects of parallel computers.

With research students, M. K. Bane and J. M. Bull, I have continued studies of asynchronous iterative algorithms. Standard iterative algorithms incur significant synchronisation delays on a parallel computer, whereas asynchronous algorithms avoid these delays, usually at the expense of a reduction in the rate of convergence of the algorithm. We have been able to characterise asynchronous polynomial zero-finding algorithms quite closely. We have also been able to identify a class of systems of linear equations for which an asynchronous Jacobi iteration converges more rapidly than its synchronous counterpart.

Also with J. M. Bull I have developed a parallel globally adaptive quadrature algorithm. It is straightforward to parallelise locally adaptive quadrature, although the algorithm has load balance difficulties for any but the most straightforward integrands. On the other hand globally adaptive quadrature is naturally sequential and it requires a modification to the underlying algorithm to enable it to be parallelised successfully. Our resulting algorithm performs well on the 32-processor KSR1 computer in the Centre for Novel Computing.

Appointments

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

Professional Activities

Editor, Advances in Computational Mathematics.

Joint convenor of the minisymposium “Parallelism in Numerical Methods”. LMS Durham Symposium on Evolutionary Problems, University of Durham, July 1992.

Publications

T. L. Freeman and C. Phillips. **Parallel Numerical Algorithms**. 315 pages. Prentice Hall International Series in Computer Science, New York, May 1992.

J. M. Bull and T. L. Freeman. *Numerical Performance of an Asynchronous Jacobi Iteration*. Pp. 361–366, **Parallel Processing: CONPAR 92–VAPP V**, ed. L. Bougé, M. Cosnard, Y. Robert and D. Trystram, Lecture Notes in Computer Science Vol. 634, Springer-Verlag, Berlin, September 1992.

Lectures

“Asynchronous iterative algorithms”. Seventh International Workshop on The Use of Supercomputers in Theoretical Science, University of Antwerp, June 1992.

“Asynchronous Jacobi iterations”. Fifth SERC Numerical Analysis Summer School, University of Lancaster, July 1992.

“Numerical Performance of an Asynchronous Jacobi iteration”. CONPAR 92–VAPP V, Lyon, September 1992. (Talk presented by J. M. Bull).

“Parallel Numerical Computing”. Manchester Centre for Computational Mathematics, University of Manchester, December 1992.

Research Grants

Investigator in collaborative grant funded by ESPRIT Basic Research Action Programme, titled “Performance-critical Applications of Parallel Architectures” (APPARC). Involves nine European institutions. Manchester group headed by Prof. J. Gurd, Computer Science; approximately £157,000 over three years, starting April 1992.

Project Co-ordinator of the project “Recursive Parallel Algorithms for Numerical Computation”, funded by the NATO Collaborative Research Grant ref. no. CRG.920037 from May 1992.

G. Hall

Senior Lecturer
Ph.D. University of Manchester, 1968

I have continued my work on adaptive algorithms and stability for initial-value problems in ordinary differential equations. The immediate practical aim is to derive robust strategies for controlling the integration which will prevent step rejections and eliminate unwanted nonsmooth behaviour of the discrete solution. It is also interesting to investigate novel control strategies which will be more effective in suppressing other types of spurious behaviour.

This work is at an advanced stage with respect to Runge–Kutta codes and is beginning for other types of methods. I am also testing the ideas in the area of Runge–Kutta codes for delay equations.

Appointments

Course Director. M.Sc. in Numerical Analysis and Computing.

Mathematics representative on the Science Faculty Postgraduate Committee.

Senior Postgraduate Tutor, Department of Mathematics.

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

Publications

D. J. Higham and G. Hall (1992). *Runge–Kutta equilibrium theory for a mixed relative/absolute error measure.* **Proceedings of the International Conference on Computational ODEs,** London, England, eds., J. R. Cash and I. Gladwell, pp. 73–85.

G. Hall (1992). *A modified stepsize strategy for algorithms based on explicit Runge–Kutta methods.* In **Computational Ordinary Differential Equations** ed. S. O. Fatunla, 109–115, University Press PLC, Ibadan. Proceedings of the Third International Conference on Computational Mathematics, Benin, Nigeria.

Conferences

The Durham Symposium on Evolutionary Problems, Durham, June 1992. (This visit was paid for by a grant from SERC.)

Nicholas J. Higham

Reader

Ph.D. University of Manchester, 1985

During the year my work on numerical stability in matrix computations continued in several areas. With J. W. Demmel and R. S. Schreiber I investigated the stability of block LU factorization, showing that the backward error depends on the condition number and a growth factor. Even for symmetric positive definite matrices, block LU factorization can be unstable, but for matrices that are block diagonally dominant by columns, stability is assured.

With Ph.D. student P. A. Knight I examined the stability of stationary iterative methods for solving singular systems. We obtained conditions under which a stationary iterative method is forward stable or backward stable. The component of the forward error in the null space of the coefficient matrix can grow linearly with the number of iterations, but it is innocuous as long as the iteration converges reasonably quickly.

Following on from my earlier work on condition numbers and backward error for structured linear systems I considered the Sylvester equation $AX - XB = C$. I obtained an expression for the backward error of an approximate solution Y; it shows that, unlike for linear systems $Ax = b$, the backward error can exceed the relative residual by an arbitrary factor. I also derived a sharp perturbation bound; the condition number it defines can be arbitrarily smaller than the $\mathrm{sep}(A, B)^{-1}$-based quantity that is usually used to measure sensitivity. I wrote a Fortran 77 code `dggsvx` that implements my error bounds; it will appear as a driver in a future release of LAPACK.

With A. Pothen I considered a parallel method for solving sparse triangular systems with many right-hand sides. We showed that while the method can be unstable, stability is guaranteed if a certain scalar that depends on the matrix and the partition is small, and that this scalar is small when the matrix is well-conditioned. Moreover, under suitable assumptions on the method, the backward error matrix can be taken to be sparse.

During the year I researched and wrote a book *Handbook of Writing for the Mathematical Sciences*, to be published by SIAM in June 1993. It grew out of notes for a short lecture course on mathematical writing that I gave to graduate students at Manchester in May 1992.

Appointments

Senior visitor at the Institute for Mathematics and its Applications, University of Minnesota, January–March 1992 (winter quarter of the IMA's Applied Linear Algebra year).

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

Numerical Analysis seminar organizer.

Professional Activities

Editor, SIAM Journal on Matrix Analysis and Applications.

Guest editor for special issue of Linear Algebra and its Applications in honour of Marvin D. Marcus (in process).

SIAM News representative of SIAM Activity Group on Linear Algebra.

"Local expert" for week on Large Scale Matrix Problems in fifth SERC Numerical Analysis Summer School, Lancaster University, July 1992.

Referee for ten journals.

Publications

(Most of these publications are available by anonymous ftp from `vtx.ma.man.ac.uk` `(130.88.16.2)` in `pub/higham`. See the `README` file therein.)

J. W. Demmel and N. J. Higham. Stability of block algorithms with fast level-3 BLAS. *ACM Trans. Math. Soft.*, 18(3):274–291, Sept. 1992.

J. W. Demmel, N. J. Higham, and R. S. Schreiber. Block *LU* factorization, Numerical Analysis Report No. 207, University of Manchester, February 1992. Submitted to *Journal of Numerical Linear Algebra with Applications*.

J. J. Du Croz and N. J. Higham. Stability of methods for matrix inversion. *IMA Journal of Numerical Analysis*, 12:1–19, 1992.

D. J. Higham and N. J. Higham. Backward error and condition of structured linear systems. *SIAM J. Matrix Anal. Appl.*, 13(1):162–175, Jan. 1992.

D. J. Higham and N. J. Higham. Componentwise perturbation theory for linear systems with multiple right-hand sides. *Linear Algebra and Appl.*, 174:111–129, 1992.

N. J. Higham. Estimating the matrix p-norm. *Numer. Math.*, 62:539–555, 1992.

N. J. Higham. Stability of a method for multiplying complex matrices with three real matrix multiplications. *SIAM J. Matrix Anal. Appl.*, 13(3):681–687, July 1992.

N. J. Higham. Perturbation theory and backward error for $AX - XB = C$. Numerical Analysis Report No. 211, University of Manchester, England, April 1992. To appear in BIT.

N. J. Higham. The joy of anonymous FTP. *IMA Numerical Analysis Newsletter*, 17(1):61–64, October 1992.

N. J. Higham and P. A. Knight. Finite precision behaviour of stationary iteration for solving singular systems. Numerical Analysis Report No. 215, University of Manchester, June 1992. To appear in *Linear Algebra and Appl.*, special issue for Proceedings of Workshop on Computational Linear Algebra in Algebraic and Related Problems.

N. J. Higham and A. Pothen. Stability of the partitioned inverse method for parallel solution of sparse triangular systems. Numerical Analysis Report No. 222, University of Manchester, England, October 1992; to appear in *SIAM J. Sci. Comput.*

Fortran 77 condition estimation routine `xLACON` in LAPACK 1.0 (1992).

Lectures

Estimating the Matrix p-norm. Institute for Mathematics and Its Applications, University of Minnesota, January 1992.

Componentwise error analysis for stationary iterative methods. Workshop on Linear Algebra, Markov Chains, and Queuing Models, Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, January 1992.

Block matrix algorithms: Stable or Unstable? Advanced Computing Research Institute, Cornell University, April 1992.

Finite precision behaviour of stationary iteration for solving singular systems. Workshop on Computational Linear Algebra in Algebraic and Related Problems, Institute for Experimental Mathematics, University of Essen, Germany, July 1992.

Parallel eigenvalue computations via matrix multiplication and inversion. Second Workshop on Parallel Numerical Analysis, Edinburgh Parallel Computing Centre, University of Edinburgh, June 1992.

Parallel eigenvalue computations via the matrix sign function. Fifth SERC Numerical Analysis Summer School, Lancaster University, July 1992.

Perturbation theory and backward error for $AX - XB = C$. NATO Advanced Study Institute on Linear Algebra for Large Scale and Real-Time Applications, Kathiolieke Universiteit Leuven, Belgium, August 1992.

——. Northern Universities' Numerical Analysis Colloquium, Leeds, September 1992.

Open Problems in Parallel Numerical Linear Algebra. Manchester Centre for Computational Mathematics, University of Manchester, November 1992.

Open Problems in Parallel Numerical Linear Algebra, and Componentwise Analysis for Linear Equations. Institute of Information Processing, University of Umeå, Sweden. November 1992.

Research Grants

One Year Science Research Fellowship from the Nuffield Foundation, 1991/1992. (value £18,264 for replacement lecturer, £1290 for research expenses).

Principal investigator on project "Numerical Stability in Matrix Computations" funded by SERC for three years from October 1992 (value £8505). Grant GR/H52139.

Investigator in collaborative grant funded by ESPRIT Basic Research Action Programme, titled "Performance-critical Applications of Parallel Architectures" (APPARC). Involves nine European institutions. Manchester group headed by Prof. J. Gurd, Computer Science; approximately £157,000 over three years, starting April 1992.

David J. Silvester

Lecturer
Ph.D. University of Manchester, 1984

During the year my research in the design of efficient algorithms for solving the incompressible Navier-Stokes equations continued. My joint work with Andy Wathen on the analysis of preconditioned Conjugate Residual methods for solving symmetric indefinite Stokes problems was particularly noteworthy. Building on our earlier work on diagonal preconditioners we went on to analyse a range of more sophisticated approaches; incomplete factorisations and fast Poison solvers were studied in detail. Our theoretical results apply to stable approximations of the Stokes operator, typically based on staggered grids, and also to recently developed *stabilised* approximations; equal order finite element methods, or finite difference methods on unstaggered grids.

One of my Ph.D. research students, John Atanga, successfully submitted his thesis over the summer. John's thesis was an analysis of three well known iterative approaches for solving the Stokes system referred to above. The mixed finite element approximation that John was primarily interested in was the bilinear velocity–constant pressure Q_1–P_0 quadrilateral. This approximation method is infamous for being unstable in the standard Galerkin formulation, so that without stabilisation all iterative solution approaches are doomed to failure. John's work showed that this difficulty can be circumvented using the local stabilisation approach that I had developed with a previous Ph.D. student; Nasserdine Kechkar. Indeed John's results show that when appropriately stabilised all iterative Stokes solvers behave as they would when using an a-priori stable method. John's thesis also contains some interesting theoretical results on the "optimal" choice of stabilisation parameter, and some preliminary calculations using a two-level hierarchical preconditioner for the Laplacian part of the Stokes operator.

My second Ph.D, research student, Richard Hanby also made steady progress over the year. Richard has been testing a variety of preconditioned Krylov subspace iterations in the context of a finite volume swirling flow code developed by his CASE sponsor Rolls Royce plc. Richard's aim is to replace the existing segregated (linear) solver in this code by a coupled solution approach. Our preliminary results show that a good Krylov subspace method for solving the coupled equations is the Quasi-Minimal Residual method recently developed by Freund and Nachtigal. We believe that combining QMR with an efficient preconditioner for the convection-diffusion operator will lead to a much more robust algorithm than that already in the code.

Whilst visiting Stanford University over the Summer, I continued to work with Philip Gresho from Lawrence Livermore National Labs on his book, *Incompressible Flow and the Finite Element Method*, to be published by Wiley. We are performing a detailed study of the instability of the Q_1–P_0 method referred to above. This approximation method is widely used in practice (despite its instability) and our joint analysis will form an important part of the book.

Appointments

Research Visitor at the Centre for Scientific Computing and Computational Mathematics, Stanford University, June–September 1992.

Publications

N. Kechkar and D. Silvester, Analysis of locally stabilised mixed finite element methods for the Stokes problem. *Math. Comp.* **58**, 1–10, 1992.

J. Atanga and D. Silvester, Iterative methods for stabilized mixed velocity–pressure finite elements. *Int. J. Numer. Meth. Fluids* **14**, 71–81, 1992.

A. Wathen and D. Silvester, The convergence of Krylov-space methods for the Stokes problem in computational fluid dynamics, University of Bristol Report, AM–92–03; submitted to *SIAM J. Sci. Stat. Comput.*

D. Silvester and A. Wathen, Fast iterative solution of stabilised Stokes systems part II: using block preconditioners, MCCM Report No. 218, July 1992; submitted to *SIAM J. Num. Anal.*

D. Silvester, Optimal low order finite element methods for incompressible flow, MCCM Report No. 223, December 1992; submitted to *Comp. Meths. Appl. Mech. Eng.*

Lectures

Symmetric and non-symmetric conjugate gradients on parallel processing computers, Manchester Centre for Computational Mathematics, January 1992.

Finite elements and parallel processing parts I and II, presented at a short course on "Parallel Computing for Finite Element Methods in Solid Mechanics", University of Manchester Department of Simon Engineering, April 1992.

Fast iterative solvers for incompressible flow problems, Stanford University Centre for Scientific Computing, July 1992.

Krylov subspace methods for solving the (Navier–)Stokes equations, presented at the annual "Scottish Computational Mathematics Meeting", University of Strathclyde, September 1992.

Efficient preconditioners for incompressible flow, Oxford University Computing Laboratory, November 1992.

Yiorgos S. Smyrlis

Temporary Lecturer
Ph.D. Courant Institute, New York University, 1989

I have been working on dissipative dynamical systems, more specifically, on Kuramoto-Sivashinsky equation and variants, with Demetrius Papageorgiou, George Papanicolaou and Adrian Coward. More specifically our work depends heavily on large scale computations to investigate windows of the diffusion parameter and more particularly those windows where chaotic behaviour is experienced.

Together with D. T. Papageorgiou we started working on a new area of dissipative dynamical systems with dispersion. This work begins a full study of the evolution equations which describe two-phase interfacial flow in a circular pipe in the limit of small annular lubricating layers. These equations were derived by Papageorgiou et al., who also provided some preliminary numerical results. The trend established is that dispersion acts in a regularizing manner to organize spatio-temporal chaotic motions into steady-state travelling waves. In this work we quantify this observation by an exhaustive set of numerical experiments. Two canonical cases are of interest: the limit of strong dispersion weak dissipation, and that of strong dissipation weak dispersion. In the former case we describe the regularization of quasi-periodic in time solutions by small dissipation effects, while in the latter the effect of dispersion on routes to chaos are evaluated.

I have also being working on travelling discrete waves. The question is to establish existence, parametrization and stability of travelling shocks solutions of dispersive finite difference schemes, for example of the Lax-Wendroff scheme. This work is continuation of my Ph.D. thesis which has received new attention with the work of Hsien Wu (a student of Tai Ping Liu,) who claims to has shown nonexistence of travelling discrete shocks for the Lax-Wendroff scheme in some cases, namely when the stregth of of the shock is very small.

Publications

D. T. Papageorgiou, G. C. Papanicolaou and Y. S. Smyrlis, Modulational stability of periodic solutions of the Kuramoto - Sivashinsky equation, from “Singularities in fluids, plasmas and optics”, ed. R. Caflisch, Kluwer Academic Publishers, Netherlands (1992).

D. T. Papageorgiou and Y. S. Smyrlis, Nonlinear dissipative dispersive waves in core annular flows, in Proceedings of NATO Advanced Workshop, Institute for Applied and Computational Mathematics, Heraklion, Crete, July 1992.

Lectures

Presented a seminar at the Courant Institute, New York University, April 1992.

Presented a series of ten lectures on Navier-Stokes Equations at the department of Mathematics, University of Manchester, May 1992.

Presented a paper with co-author D.T.Papageorgiou at the NATO Advanced Research Workshop, Heraklion, Crete, July 1992.

Conferences

Courant Institute, April 1992.

NATO Advanced Research Workshop, Crete, July 1992.

Research Grants

NATO travel grant of $5000 (joint with D. T. Papageorgiou) since May 1992 (2 years duration.)

R. W. Thatcher

Senior Lecturer
PhD University of London, 1972

My main research activity during 1992 was domain decomposition and parallel algorithms for solving partial differential equations. Much of this work was done in collaboration with M. A. Leschziner; a jointly supervised research assistant, D. Golby, was doing work on a parallel implementation of an Euler code to compute flow around an aerofoil and a research student, B. Tanyi, was doing similar work with the TEACH code for incompressible flows. The results of this work were presented at an ERCOFTAC meeting on Domain Decomposition at Leeds University in September 1992. Additionally with two research students, P. Lockey and C. Rostron, research on parallel preconditioning using domain decomposition for elliptic equations was carried out.

Work was continued on my two other main research interests, finite element techniques for approximating fluid flow and approximating singularities. Work on the former area included writing a chapter for a book *Recent Advances in Computational Fluid Dynamics* edited by R. A. Nicolaides and M. Gunzburger to be published by Cambridge University Press in 1993. The work on the latter area will be presented, by invitation, at an international workshop at CIRM, France in 1993.

Appointments

Deputy Chairman of Mathematics Department, UMIST.

Deputy Director of MCCM.

University responsibilities include: Head of Numerical Analysis Group (UMIST); Membership of Academic Establishment Committee, Appraisal Working Party at UMIST, Dean's Working Party on Modularisation and Semesterisation; Chairman of Board of Studies for Mathematics and Management Sciences Course.

Publications

B. A. Tanyi and R. W. Thatcher, On the parallelisation of the TEACH-T code for computing fluid flow, Numerical Analysis Report No. 216, University of Manchester, June 1992; to appear in Proc. 1992 Edinburgh Symposium on Parallel Computing.

P. Lockey and R. W. Thatcher, Efficient implementation of preconditioned conjugate gradients on a transputer network, Numerical Analysis Report No. 217, University of Manchester, June 1992; to appear in Proc. 1992 Edinburgh Symposium on Parallel Computing.

Lectures

Domain decomposition; a parallel algorithm for preconditioning. Manchester Centre for Computational Mathematics, University of Manchester, October 1992.

Research Grants

In collaboration with Professor Leschziner in Mechanical Engineering at UMIST we have a three year grant for £62K for a postdoctoral research assistant to make a study of domain decomposition and parallel methods. The aim is to implement such techniques into existing CFD codes on a computer with a parallel architecture. The project was started in April 1991 when Dr D Golby was appointed as Research Assistant.

Ruth M. Thomas

Senior Lecturer elect
Ph.D. University of Manchester, 1979

During the year, I continued to work on the numerical solution of differential/algebraic boundary value problems in collaboration with my former research student, C. C. Beardah, and with colleagues at ICI plc, who have a specific interest in problems of this type, arising in the modelling of detonation. I devised and developed several numerical techniques for solving these problems and investigated the advantages and disadvantages (both theoretical and practical) of each approach. The software produced is now being used by ICI plc. It is general purpose and is capable of solving a wide range of general differential/algebraic boundary value problems.

Following my earlier work on deriving and analysing the properties of numerical methods for solving pure oscillation problems, I derived and developed efficient algorithms and computer software for solving such problems.

My duties as Secretary of the Organising Committee of the LMS Symposium on Evolutionary Problems continued to take up a great deal of time and effort during the first seven months of the year. I had taken on this role early in 1990 and shared the major administrative burden with Professor Christopher Baker of the University of Manchester. The 10-day Symposium took place in July 1992 and was attended by over 90 mathematicians from all over the world.

Professional Activities

Secretary of the Organising Committee for the 1992 LMS Durham Symposium on Evolutionary Problems.

Referee for numerous journals.

Publications

M. S. H. Khiyal and R. M. Thomas. Efficient P-stable methods for second order systems. In: *Proceedings of the IMA Conference on Computational Ordinary Differential Equations* (edited by J.R. Cash and I. Gladwell), pages 127-134, OUP, 1992

C. C. Beardah and R. M. Thomas. Two mathematical models of unconfined detonation and their numerical solution. To appear in: *Circuits, Systems and Signal Processing*

C.C. Beardah and R.M. Thomas, Collocation Techniques for Solving Mathematical Models of Unconfined Detonation, Numerical Analysis Report No. 219, University of Manchester, September 1992.

R. M. Thomas and M. S. H. Khiyal, High order P-stable methods for nonlinear oscillation problems, Numerical Analysis Report No. 221, University of Manchester, October 1992.

Lectures

C. C. Beardah and R. M. Thomas. The Numerical Solution of Differential/Algebraic Boundary Value Problems Arising in Detonation Theory. SIAM 40th Anniversary Meeting, Los Angeles, July 1992. (Talk presented by C. C.Beardah.)

Conferences

The LMS Symposium on Evolutionary Problems at the University of Durham, 4th-14th July 1992. (All my expenses were paid by a grant from the SERC.)

Joan E. Walsh

Professor and Pro-vice chancellor
D.Phil., Oxford University, 1959

I am on secondment as a Pro-vice chancellor, but retain my interest in the numerical analysis of partial differential equations and in numerical modelling of industrial problems.

Appointments

Pro-vice chancellor with special responsibility for teaching.

Vice-President, Institute of Mathematics and its Applications

Member of Council, Numerical Algorithms Group Ltd., Oxford.

President, National Conference of University Professors.

Publications

J. Walsh et al., The future for honours degree courses in mathematics and statistics, IMA Bulletin, 28 (4/5), pp. 81–91, 1992.

Jack Williams

Lecturer
D.Phil. University of Oxford, 1968

During the year I have given most attention to research on approximation from parameter-dependent ordinary differential equations. This has been from the approximation theory viewpoint but motivated by the application to the parameter estimation problem for single equation models. Certain classes of differential equations have been identified whose solutions yield unique global best Chebyshev approximations. This is in contrast to least squares fitting where it does not appear possible to say if a computed best fit is a unique global best approximation.

I have also been collaborating with Dr. S. D. R. Wilson of the applied mathematics group on the numerical solution of a 4th order partial differential equation (of initial-value type) which models the Drag–problem. An interface condition involving discontinuities has lead by the method of lines to an differential-algebraic system.

Professional Activities

Secretary, panel session on parallel computation, NATO Advanced Research Workshop Algorithms for Approximation 1992, Lady Margaret Hall, Oxford, July 1992.

Chairman, session on applications of approximation, NATO Advanced Research Workshop Algorithms for Approximation 1992, Lady Margaret Hall, Oxford, July 1992.

Referee for SERC grant application.

External Examiner for a Ph.D. Thesis and Internal Examiner for a Ph.D. Thesis.

Publications

Jack Williams and Z. Kalogiratou *Best Chebyshev approximation from families of ordinary differential equations.* **IMA J. Numer. Anal.**. To appear.

Jack Williams and Z. Kalogiratou (1993) *Nonlinear Chebyshev fitting from the solution of Ordinary Differential Equations.* **Advances in Computational Mathematics.** To appear.

Lectures

Parameter estimation and approximation in ODE's. London Mathematical Society Durham Symposium on Evolutionary Problems, University of Durham, July 1992.

Nonlinear Chebyshev fitting from the solution of ODE's. Conference on Algorithms and Approximation III, NATO Advanced Research Workshop, Lady Margaret Hall, University of Oxford, July 1992.

Long-Term Visitors

Graeme Sneddon

Department of Mathematics, James Cook University, Queensland
Ph.D. Monash University, 1977
July–December 1992

I am working on the eigenvalues of second-order spectral differentiation matrices, with the aim of choosing a scheme that would avoid the $O(N^4)$ growth of the largest eigenvalue. In fact a scheme has been found to achieve this, though with a slight increase in errors compared with some other schemes.

Lectures

Evaluation of tail correction integrals. Manchester Centre for Computational Mathematics, University of Manchester, November 1992.

Publications

M. J. Ridd, D. J. Gakowski, G. E. Sneddon, and F. R. Keene, Mechanism of Oxidative Dehydrogenation of Alcohols co-ordinated to Ruthenium, J. Chem. Soc. (Dalton Transactions) (1992) pp. 1949–1956.

Short-Term Visitors

K. Burrage, University of Queensland, Brisbane, Australia, July 1992.

J. C. Butcher, Department of Mathematics and Statistics, University of Auckland, New Zealand, July 1992.

Chunyang He, Department of Mathematics, Bielefeld University, Germany, September 1992.

V. B. Kolmanovskii, Russian Academy of Science, Moscow. July 1992.

K. Nafa, Department de Matematiques, Universite d'Annaba, Algeria, September 1992.

Numerical Analysis Reports

207. J.W. Demmel, N.J. Higham and R.S. Schreiber, Block *LU* factorization, February 1992.

208. C.T.H. Baker, J.C. Butcher and C.A.H. Paul, Experience of STRIDE applied to delay differential equations, January 1992.

209. D.R.Willé, Towards an alternative error control strategy for ordinary and delay-differential equations, January 1992.

210. J.M. Bull and T.L. Freeman, Numerical performance of an asynchronous Jacobi iteration, March 1992.

211. N.J. Higham, Perturbation theory and backward error for $AX - XB = C$, April 1992.

212. C.T.H. Baker and C.A.H. Paul, Explicit Runge–Kutta methods for the numerical solution of singular delay-differential equations, April 1992.

213. C.A.H. Paul, A fast, efficient, very low storage, adaptive quadrature scheme, May 1992.

214. C.T.H. Baker and R.M. Thomas, Durham symposium titles and abstracts, June 1992.

215, N.J. Higham and P.A. Knight, Finite precision behaviour of stationary iteration for solving singular systems, June 1992.

216. B.A. Tanyi and R.W. Thatcher, On the parallelisation of the TEACH-T code for computing fluid flow, June 1992.

217. P. Lockey and R.W. Thatcher, Efficient implementation of preconditioned conjugate gradients on a transputer network, June 1992.

218. David Silvester and A.J. Wathen, Fast iterative solution of stabilised Stokes systems part II: using block preconditioners, July 1992.

219. C.C. Beardah and R.M. Thomas, Collocation Techniques for Solving Mathematical Models of Unconfined Detonation, September 1992.

220. C. T. H. Baker, Stability functions for multistep formulae for Volterra functional equations, October 1992.

221. R. M. Thomas and M. S. H. Khiyal, High order P-stable methods for nonlinear oscillation problems, October 1992.

222. N. J. Higham and A. Pothen, Stability of the partitioned inverse method for parallel solution of sparse triangular systems, October 1992.

223. David Silvester, Optimal low-order finite element methods for incompressible flow. December 1992

Numerical Analysis Seminars

January 15. David Silvester (UMIST). Symmetric and non-symmetric conjugate gradients on parallel processing computers.

February 5. John Mason (RMCS). Chebyshev polynomials of the 2nd, 3rd and 4th kind—Properties and Applications.

February 12. David Griffiths (Dundee). Wave-like solutions in the approximation of PDE's.

February 19. Charles Elliott (Sussex). Numerical approximation of curvature dependent phase boundary motion.

February 26. Les Hatton (Prog. Res. Ltd.). The quality and reliability of scientific software.

March 11. Christopher Paul (Manchester). Stability regions for Runge–Kutta DDE methods

April/May. Yiorgos Smyrlis (Manchester). Analysis and numerical treatment of Navier-Stokes equations (10 lectures).

June 17. Philip Knight (Manchester). Finite precision behaviour of stationary iterative methods.

October 7. Ron Thatcher (UMIST). Domain decomposition; a parallel algorithm for preconditioning.

October 28. Christopher T. H. Baker (Manchester). Nonlinearity and memory in the numerical treatment of evolutionary (functional-)differential equations.

November 4. Nick Higham (Manchester). Open problems in parallel numerical linear algebra.

November 11. Graeme Sneddon (Queensland). Evaluation of tail correction integrals.

November 18. Chris Phillips (Newcastle). Practical exploitation of parallelism.

December 2. Sven Hammarling (NAG, Oxford). The numerical solution of the generalized symmetric eigenvalue problem.

M.Sc. Degrees

S. Bosman, Discrete Chebyshev Approximation, 1992.

D. A. Burgess, Parallel Computing of Finite Elements: Modelling Incompressible Stokes Flow, 1992.

A. P. Jackson, Solution of Poisson's Equation on 1024 Processors Using a Multigrid Approach, 1992.

K. F. Loh, Collocation Techniques for Solving Second Order IVPs in Ordinary Differential Equations, 1992.

S. M. Ramsden, Givens QR Factorization on the INTEL iPSC/2 Hypercube, 1992.

Ph.D. Degrees

John Atanga, Iterative Methods for Locally Stabilised Mixed Finite Element Methods, 1992.

Michael K. Bane, Linear Algebra and Asynchronous Polynomial Zero-Finding Algorithms for Transputer Arrays, 1992.

Christian C. Beardah, Finite Difference Solution of Differential/Algebraic Boundary Value Problems Arising in Modelling of Unconfined Detonations, 1992.

Zacharoula Kalogiratou, Problems on Nonlinear Chebyshev Approximation, 1992.

Christopher A. H. Paul, Runge–Kutta Methods for Functional Differential Equations, 1992.