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Abstracts

Section A: Invited Talks

Section B: Submitted Talks

Section A: Invited Talks

Pivoting and stability in the augmented system method

Åke Björck, Linköping University, Sweden

In many contexts it is required to solve an augmented linear system of the form

$$\begin{pmatrix} W & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} y \\ x \end{pmatrix} = \begin{pmatrix} b \\ c \end{pmatrix},$$

where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and $W \in \mathbb{R}^{m \times m}$ symmetric positive semidefinite. In the special case when $W = I_m$ this system gives the conditions for solution of both the linear least squares problem $\min_x (\|Ax - b\|_2 + 2c^T x)$ and the minimal distance problem $\min_x \|b - y\|_2$, where $A^T y = c$. Since the augmented system is symmetric and indefinite it can be solved by computing an LDL^T factorization of the augmented matrix, where D is block-diagonal with 1×1 and 2×2 pivots, using a pivoting technique due to Bunch and Kaufman.

If $\alpha > 0$ is a parameter, then an equivalent augmented system is obtained by the scaling $W := \alpha W$, $y := \alpha^{-1} y$, $c := \alpha^{-1} c$. If the Bunch-Kaufman pivoting is employed the choice of pivots and therefore the stability of the method will depend on the parameter α . For the case $W = I_m$ we derive optimal values of α based on minimizing different bounds for the round-off error in the solution. It is shown that acceptable error stability can be achieved by proper choice of α . We also consider the case when $W = \text{diag}(0_p, I_{m-p})$ which covers constrained linear least squares problems. The possible extension of the results to general weighted problems is discussed.

The augmented system approach has been successfully applied both to sparse linear least squares problems and to sparse quadratic programming. For sparse problems the pivoting strategy has to be a compromise between stability and sparsity, but accuracy of the computed solution can often be restored by iterative refinement.

Portable Numerical Software for High Performance Parallel Machines

James Demmel, University of California at Berkeley, USA.

It is difficult to write fast software for parallel machines. It is also difficult to write robust numerical software which is portable across different architectures. It is doubly difficult to do both. Nevertheless, this is the goal of the LAPACK project, which is implementing linear algebra computations. The first phase of the project targeted dense and banded linear algebra computations on shared memory machines. The second phase, which is just beginning, also includes distributed memory machines and sparse linear algebra. We discuss past progress and open problems.

A Parallel Algorithm for the Non-symmetric Eigenvalue Problem

Jack Dongarra, University of Tennessee and Oak Ridge National Laboratory, USA.

We will describe a parallel algorithm for computing the eigenvalues and eigenvectors of a non-symmetric matrix. The algorithm is based on a divide-and-conquer procedure and uses an iterative refinement technique.

Matrices, moments and quadrature

G. H. Golub, Stanford University, USA.

Given an $n \times n$ symmetric, positive definite matrix A and a real vector u , it is desirable to estimate and bound the quadratic form

$$u^T F(A) u / u^T u$$

where F is a differentiable function. This problem arises in estimating errors of linear systems, computing a parameter in a least squares problem with a quadratic constraint and bounding elements of the inverse of a matrix.

We describe a method based on the theory of moments and numerical quadrature for estimating the quadratic form. A basic tool is the Lanczos algorithm which can be used for computing the recursive relationship for orthogonal polynomials. Some numerical experiments will be described.

A personal view of large-scale nonlinear programming

Nick Gould (Rutherford Appleton Laboratory) A. R. Conn and Ph. L. Toint.

In this talk, we shall describe the numerical algorithms which lie at the heart of the large-scale nonlinear programming package, LANCELOT. The methods have been designed to allow the solution of problems with thousands of variables and constraints on a reasonable workstation. We will explain the theory, old and new, which underpins our algorithms and provide some evidence of the efficacy of our approach. We will also give some indication of future directions of research in the field

A Review of Uniform Subdivision

John A. Gregory, Brunel University

The generation of curves and surfaces by recursive subdivision will be discussed. In particular, the theory of uniform subdivision schemes will be considered and recent work in this area will be reviewed. The generation of Box-splines provides a nice illustration of the theory and interpolatory subdivision methods will also be considered.

Numerical analysis of functional equations with a variable delay

A. Iserles and Martin Buhmann, University of Cambridge.

The generalized pantograph equation

$$y'(t) = Ay(t) + By(qt) + Cy'(qt), \quad y(0) = y_0,$$

where $y \in \mathbb{C}^d$, A, B, C are $d \times d$ matrices and $q \in (0, 1)$ has numerous applications in areas as diverse as collection of current by electric locomotives, Cherenkov radiation, dielectricity, number theory and the expansion of galaxies.

The very question of well-posedness of the generalized pantograph equation is nontrivial and we commence our talk by a short review of this area. Next, we briefly discuss conditions that are required to ensure asymptotic stability and debate the behaviour of y on the stability boundary. This includes some interesting instances of fractal-like behaviour.

Although the extension of standard ODE methods to this (infinite-dimensional) dynamical system is easy, their stability analysis presents formidable difficulties, since the underlying difference equations are non-stationary. Nonetheless, the question of stability for the linear test equation

$$y'(t) = ay(t) + by(qt) + cy'(qt), \quad y(0) = y_0,$$

has been satisfactorily resolved, using techniques from Fourier analysis and ergodic theory.

The Slightly Compressible Navier-Stokes Equations
Jens Lorenz, The University of New Mexico, USA.

At low Mach numbers, the solutions of the compressible Navier-Stokes equations vary on two different time scales: The fast scale corresponds to the sound speed, the slow scale to the convective speed. If there are no boundaries, then one can decompose the solution to first order into an incompressible part and fast density/pressure fluctuations. The presence of boundaries makes this picture much more complicated if the viscous term in the Navier-Stokes equations is not neglected, because this term changes the admissible boundary conditions. The resulting mathematical difficulties have only been partially solved.

Upwinded Test Functions for Finite Element and Finite Volume Methods
K.W. Morton, University of Oxford.

Ever since the initial collaboration between Ron Mitchell and Olek Zienkiewicz in the mid-1970's, upwinding through the Petrov-Galerkin formalism has been the standard technique for adapting finite element methods to cope with the difficulties of convection-dominated flow problems. Indeed, the SUPG method (streamline upwind Petrov-Galerkin) has through the joint work of Tom Hughes and Claes Johnson in the 1980's become the best known finite element technique for this class of problem. In Barrett and Morton (1984) it was shown how these techniques can be interpreted as approximating the symmetrization of the elliptic diffusion operator, which has been made unsymmetric by the addition of convection. Moreover, this accounts for the better conditioning of the resultant discrete equations.

Over a similar period many researchers have developed finite element methods for evolutionary hyperbolic problems, in particular various types of characteristic Galerkin method. These can also be written in a form which uses an upwinded test function, although they fall outside the Petrov-Galerkin framework and the relationship with the earlier class of test functions is unclear.

By considering the unsteady convection-diffusion equation we shall show how these two strands in the development and generalisation of the Galerkin technique are related; indeed, with a particular choice of mixed norm (depending on the mesh Peclet number) they satisfy the same identity.

Finite volume methods have been steadily growing in popularity for equilibrium problems, both elliptic and hyperbolic. Derivation of the schemes is often rather ad hoc, but we discuss the use that some make of upwind control volumes and how this relates to the corresponding finite element developments.

The complexity of Karmarkar's algorithm for linear programming
M. J. D. Powell, University of Cambridge.

Karmarkar's algorithm has attracted much interest, partly because it can solve linear programming problems to prescribed accuracy in polynomial time. In other words the amount of work can be bounded above by a polynomial in n , where n is the number of variables plus the number of constraints. Specifically, this amount is dominated by the number of changes to the variables, m say, multiplied by the computation time of a typical change. Further, when the algorithm was first proposed it was known that m is at most a constant multiple of n . Several variations on the original algorithm have been developed from its relation to the logarithmic barrier function method for constrained optimization

calculations. Thus one can achieve the condition $m = O(n^{1/2})$, which raises the question whether the original algorithm also enjoys this property. This work will be surveyed, and the question will be answered by an example which shows that $m > n/8$ occurs in a case where the prescribed accuracy is undemanding. Therefore the "log barrier" developments have provided substantial improvements to the usual theoretical measure of efficiency, although many practical calculations have failed to indicate this property.

Variable steps for symplectic integrators

J. M. Sanz-Serna and M. P. Calvo, Universidad de Valladolid, Spain

There has been much recent interest in the numerical integration of Hamiltonian systems of differential equations by means of so-called symplectic integrators. Many experiments have been reported in the literature which show that fixed-step implementations of symplectic formulae improve (often substantially) on fixed-step implementations of formulae like the 'classical' Runge-Kutta method. However it is reasonable to ask (i) whether the simple fixed-step symplectic formulae considered so far in the literature may improve on modern variable-step codes and (ii) whether symplectic formulae may be advantageously incorporated into a variable-step algorithm. Most numerical analysts would think that the answer to (i) should be no and the answer to (ii) should be yes.

In the talk we shall explain the meaning of 'symplectic' and report on our experience with the construction and assessment of variable-step symplectic integrators. Numerical experiments will be reported which do not back any expectations we had at the beginning of the project.

Nonlinear Parameter Estimation: Models, Criteria, Algorithms

Hubert Schwetlick, Martin Luther University, Germany

Estimating parameters p in nonlinear model equations from observations of state variables z which are subject to errors is a basic task in applied mathematics. The classical case is nonlinear regression where the model $y = r(x, p)$ with $z = (x, y)$ is explicit, the x -parts are supposed to be free of errors, and p is estimated by minimizing the y -deviations in the least squares sense. In recent time, several extensions and generalizations of this standard estimation problem have been investigated concerning

- the type of the model equation
 - + "models with separated variables" where certain of the parameters occur linearly and can be eliminated what, however, increases the complexity of the model
 - + "implicit models" $f(z, p) = 0$ that leads to highly structured problems with equality constraints and a large number of variables to be estimated
- the character of the errors
 - + "error-in-variables models" where all state variables are allowed to have errors, sometimes also called "orthogonal regression" or "total approximation problems"
- the type of the criterion function that defines the amount of the individual deviations

- + Instead of the classic quadratic criterion so called "robust" functions as the famous Huber function which are smooth but do not grow as quickly can be used. The corresponding "robust estimations" are useful when the data contain outliers.
- + A further alternative way based on a different statistical background is "multiresponse parameter estimation" where the objective function is a determinant.

The extensions mentioned above will shortly be introduced, the arising unconstrained and equality constrained optimization problems will be discussed, and appropriate solution techniques that are influenced by general optimization techniques but exploit the special structure of the problems will be described.

Unconventional methods for boundary integral equations in the plane

Ian H. Sloan, University of New South Wales, Australia.

The traditional methods for the solution of boundary integral equations are the Galerkin and collocation methods. This talk introduces some less familiar methods, characterised by unconventional quadrature rules. One is the quallocation method, a generalisation of the collocation method in which the order of convergence is increased. Another is a method which is similar in principle but fully discrete, and hence easily implemented.

Numerical methods for hyperbolic integro-differential equations

Vidar Thomée, Chalmers University of Technology, Sweden.

Stability and error estimates are derived for fully discrete numerical methods for time-dependent partial integro-differential equations of hyperbolic type. Special attention is paid to the storage requirements in the time-stepping.

Non-Normal Matrices and Pseudospectra

Lloyd N. Trefethen, Cornell University, USA.

The notion of eigenvalues developed historically in connection with problems such as heat conduction in a bar, oscillation of a drum, and energy states of a quantum mechanical system. The operators that arise in such problems are self-adjoint or skew-adjoint, hence *normal* — i.e., having orthogonal eigenfunctions. Thus the eigenfunctions form a well-behaved basis in which to expand more general functions, and statements about eigenvalues, being implicitly related to that basis, have a natural physical meaning.

All of this changes for operators or matrices that are far from normal. The spectrum can still be defined mathematically, but it may have very little to do with the operator's behavior. Examples of highly non-normal operators and matrices arise all over numerical analysis. This talk will describe the difficulties of conventional spectral analysis for such applications and survey the uses of the alternative notion of *pseudospectra*.

Analysis of an adaptive finite-difference method for time dependent PDEs

J. G. Verwer and R. A. Trombert, CWI, Amsterdam.

The subject of this lecture concerns the solution of time dependent PDEs by means of adaptive finite-difference methods. We will show how, for a conceptually simple finite-difference method, based on the techniques of locally-uniform-grid-refinement and static regridding, the spatial-grid adaptation can be analysed. Local-uniform-grid-refinement (LUGR) is an adaptive-grid technique for computing solutions of PDEs possessing sharp

spatial transitions. Using nested, finer-and-finer uniform sub-grids, the LUGR technique refines the space grid locally around these transitions so as to avoid discretization on a fine grid covering the entire physical domain. For time dependent problems the LUGR technique is easily combined with static regridding. Static regridding means that in the course of the time evolution the space grid is adapted only at discrete values of time. Our analysis leads to a local-refinement theory underlying the criterion that the multi-level LUGR method maintains the spatial accuracy of the finest grid in use when applied in the common single-grid mode. This way we automatically provide control on the inevitable accumulation of interpolation errors for evolving in time. Following the method of lines approach, we first discuss this theory for the implicit Euler LUGR method applied to a general, semi-discrete PDE problem. We next point out how results can be extended to Runge-Kutta and linear multi-step methods. The local refinement theory will be numerically illustrated for some model parabolic problems.

Section B: Submitted Talks

New Members of the Broyden Family of Formulae

M. Al-Baali, Ajman University College, UAE.

Recently, there has been an increasing interest in the self-scaling Broyden family of formulae. These formulae are usually defined by replacing the approximate Hessian matrix B by τB , where τ is a scaling parameter, in the Broyden family of formulae, which update B to obtain a new approximation to the Hessian matrix. It is clear that if B is replaced by $1/\tau B$ in a self-scaling formula, for some scaling τ , then a member of the Broyden family follows. The speaker will show in certain cases that this member is not uniquely defined. He will illustrate this point by addressing new members of the Broyden family. These members are defined simply and satisfy the usual condition, which maintains the current Hessian approximation positive definite. Because comparison with the BFGS method shows promising numerical results, the corresponding new methods are useful.

Moving Finite Elements, Approximate Characteristics and a.e. Best Fits with Adjustable Nodes

M.J. Baines, University of Reading.

The Moving Finite Element procedure for the PDE $u_t = Lu$ is

$$\min \|U_t - LU\|_2$$

over both the (linear) finite element amplitude and nodal speeds.

It is shown that for certain classes of PDEs in 1-D these speeds are a combination of approximate characteristic velocities (where they exist) and velocities obtained from an algorithm for finding a.e. best fits to the PDE solution with adjustable nodes. The extension to higher dimensions is discussed.

Error Analysis of Update Methods for the Symmetric Eigenvalue Problem

Jesse L. Barlow, The Pennsylvania State University, USA

Cuppen's divide-and-conquer method for solving the symmetric tridiagonal eigenvalue problem has been shown to be very efficient on shared memory multiprocessor architectures.

In this paper, we resolve some error analysis issues concerning this method. We show that the method is stable and suggest a slightly different stopping criterion for finding the roots of the spectral function.

These error analysis results extend to general update methods for the symmetric eigenvalue problem. That is, we have good backward error bounds for methods to find the eigenvalues and eigenvectors of $A + \rho w w^T$ given those of A . These results can also be used to analyze a new fast method for finding the eigenvalues of banded, symmetric Toeplitz matrices.

Finite Element Approximation of the P-Laplacian

John W. Barrett and W.B. Liu, Imperial College.

In this talk we consider the continuous piecewise linear finite element approximation of the following problem: Given $p \in (1, \infty)$, f and g ; find u such that

$$\begin{aligned} -\nabla \cdot (|\nabla u|^p - 2\nabla u) &= f \text{ in } \Omega \subset \mathbb{R}^2, \\ u &= g \text{ on } \partial\Omega. \end{aligned}$$

For sufficiently regular solutions u , achievable for a subclass of data f, g and Ω , we improve on the error bounds in the norm $W^{1,q}(\Omega)$; $q = p$ for $p < 2$ and $q \in [1, p)$ for $p > 2$; to be found in the literature. Numerical results demonstrating these bounds are also presented.

Dynamics of the QR algorithm.

Steve Batterson, Emory University, USA.

We consider various versions of the QR algorithm for approximating the eigenvalues of a real Hessenberg matrix. Questions concerning convergence of these algorithms are formulated as problems in dynamical systems. We indicate how these techniques can be applied in certain very special cases to understand the global convergence of Francis shifted QR and its EISPACK implementation. Another consequence of this approach is the failure of Rayleigh Quotient Iteration for sets of positive measure.

Collocation Techniques for Differential/Algebraic Boundary Value Problems

C.C. Beardah, UMIST.

We shall consider the application of a class of implicit Runge-Kutta methods to a differential/algebraic boundary value problem. We shall consider in particular the Gauss, Radau and Lobatto rules, which are collocation schemes. We shall discuss the advantages and disadvantages of these schemes and their implementation. Finally, we shall use the resulting code to solve a parameterised free boundary value problem arising in the modelling of detonation.

Transformation of Integrands for Lattice Rules

Marc Beckers and Ann Haegemans, Katholieke Universiteit Leuven.

In recent years a great amount of work is done searching for, what are called, good lattice rules. Lattice rules are used for the numerical integration of smooth functions over the unit s -dimensional cube I^s . The integrand has to be periodic with period 1 with respect to each coordinate separately. If we want to use these lattice rules in practice, it is not only important to search for good lattice rules but also to look after methods for periodizing functions. There are different ways of transforming a given integrand into a periodic one while preserving regularity properties and the value of the integral, though this has to be done at the expense of further calculations. We test the influence of transformations on different functions. We used the package of Genz for testing multidimensional integration routines based on performance profiles.

Finite Difference Schemes for Fourth-order Two-point Boundary-value Problems based upon Mixed Interpolation

G. Vanden Berghe (University of Gent, Belgium), M. Van Daele and H.E. De Meyer

The following typical fourth-order ODE problems are considered

$$\begin{aligned} y^{(4)} + f(x)y(x) &= g(x) \\ y(a) - A_1 &= y'(a) - A_2 = 0 \\ y''(b) - B_1 &= y'''(b) - B_2 = 0 \\ y^{(4)} - \lambda q(x)y(x) &= r(x)y(x) \\ y(a) = y(b) = y'(a) &= y'(b) = 0 \end{aligned}$$

Finite difference schemes are developed by using mixed interpolation functions of the type $a \cos kx + b \sin kx + \sum_{i=0}^{n-2} c_i x^i$. Due to the presence of the parameter k the numerical method can be optimized; the accuracy of the obtained results is much higher than the one obtained by the classical methods based on polynomial interpolation. For a few examples the results are briefly summarized to demonstrate the practical usefulness of the method. For the eigenvalue problem (2) it will be shown that the use of a parallel computer system can result in a significant time saving.

For ODEs, the condition (stability) of the spectral Čebyšev methods is not a problem
 Jean-Paul Berrut, Université de Fribourg, Switzerland.

As the spectral methods become increasingly recognized methods for solving differential equations, the condition of the algebraic problems they involve is given more attention. For ODEs, several authors (Funaro, Greengard,...) have noticed the large condition numbers of the arising systems of equations. Preconditioners have been presented. In a former article, we have suggested the Čebyšev spectral method *with preliminary transform to the circle* as a means of avoiding the squaring of the condition number as compared with the Fourier method. Greengard has suggested the spectral *integration* method as leading to presumably better conditioned algebraic problems.

Unfortunately, despite those large condition numbers, we could not find any example of bad behaviour of spectral methods for ODEs in the literature.

In this talk, we demonstrate with several examples that the condition number does not seem to be a real issue for the solution of ODEs (as opposed to the solution of hyperbolic or parabolic PDEs): the condition of the matrix is a bad indication of the condition of the problem.

All methods give comparable results with very smooth problems; however, the spectral integration method is probably less good than the spectral differentiation methods for not very smooth problems, since it approximates the second derivative of the unknown function instead of the unknown itself.

Finally, we show how in many cases the systems arising from the Čebyšev method with preliminary transform to the circle can be solved efficiently by iterative methods.

Fast Direct and Iterative Solvers for Orthogonal Spline Collocation Equations
 B. Bialecki, G. Fairweather and K. R. Bennett, University of Kentucky, U.S.A.

Fast direct and iterative methods are presented for the solution of linear systems arising when orthogonal spline collocation with piecewise Hermite bicubics is employed for the approximate solution of the Dirichlet problem for Poisson's equation in a rectangle. On an $N \times N$ partition, the direct method, which is the matrix decomposition algorithm involving fast Fourier transforms, requires $O(N^2 \log N)$ arithmetic operations. On the other hand, the cost of the iterative Alternating Direction Implicit method, with Jordan's selection of the acceleration parameters, is $O(N^2 \log^2 N)$. Both matrix decomposition and Alternating Direction Implicit methods are highly modular and well suited for parallel computation. Extensions of the methods to more general boundary value problems with mixed and periodic boundary conditions, as well as generalizations to higher degree piecewise polynomial spaces are discussed. The results of numerical experiments are also presented.

Fitting of Variogram Functions Generated by the Hankel Transform

J.D. Botha, University of South Africa.

Variogram functions play an important role in an estimation technique known as kriging, which is used by geostatisticians in their analysis of geostatistical data. A general class of such variogram functions can be generated by the Hankel transform. In this presentation we discuss some of the difficulties which arise in the development of an algorithm for the least squares fitting of a suitable variogram function from this class to a given set of experimental data.

Diagonally Implicit Multi Stage Integration Methods for Ordinary Differential Equations

J. C. Butcher, University of Auckland, New Zealand.

The methods discussed in this paper, which we will refer to briefly as DIMSIMs, are motivated by a consideration of the competing advantages of various existing classes of methods. The hope is that the low implementation costs, as for linear multistep methods, can be combined with good stability and high accuracy, as for Runge-Kutta methods. If this can be done we will have found methods which enjoy a combination of advantages not available in standard existing methods.

The class of methods known as general linear methods are specialised to DIMSIMs by requiring a diagonally implicit form for the matrix which corresponds to the usual matrix of coefficients in Runge-Kutta methods and by narrowing the definition of order in such a way as to ensure that efficient starting methods are available. There are actually four distinct subclasses of DIMSIMs which have specific application areas depending on whether the method is intended for stiff or non-stiff problems or whether it is to be implemented on a conventional or on a parallel computer.

Examples will be given of each of these subclasses of DIMSIMs, together with their stability and other characteristic features. The discussion of the individual methods also deals with such practical questions as local truncation error estimation, dense output and change of stepsize.

A Range of Numerical Approaches to the Nonlinear Burgers' Equation

J. Caldwell, City Polytechnic of Hong Kong.

Burgers' equation often arises in the mathematical modelling used to solve problems in fluid dynamics involving turbulence because of its similarity to the Navier-Stokes equation. Difficulties have been experienced in the past in the numerical solution of this equation, namely

$$u_t + u u_x = Re^{-1} u_{xx},$$

particularly for large Reynolds number Re which corresponds to steep fronts in the propagation of dynamic waveforms.

This paper summarises and comments on a number of numerical approaches to Burgers' equation used by the author over the past 10 years. These include finite-difference methods and a Fourier series approach which produce reasonable accuracy for small Reynolds number. Here comparison can be made with the analytical solution.

Another possible numerical technique discussed is the use of a variational-iterative scheme based on complementary variational principles.

A spectral collocation and path-following method for studying reaction-diffusion equations
J.M.Cameron, Heriot-Watt University.

We describe a spectral collocation and path following method for studying the steady state solutions of reaction diffusion problems as a function of the problem parameter. We give a specific example of the method applied to a system of coupled reaction diffusion equations

$$\begin{aligned}u_t(x, t) &= d_1 \Delta u(x, t) + \alpha f(u, v) \\v_t(x, t) &= d_2 \Delta v(x, t) + \alpha g(u, v)\end{aligned}$$

with Neumann boundary conditions, where α is the problem parameter, in both one and two space dimensions.

Symmetrizers for symmetric Runge-Kutta methods

R.P.K. Chan, University of Toronto, Canada and University of Auckland, New Zealand.

Symmetric Runge-Kutta methods are known to possess asymptotic error expansions in even powers of the stepsize for the numerical solution of ordinary differential equations. This important property provides the basis for the construction of extrapolation methods, and advantage had been taken in the development of codes for stiff problems that use the implicit midpoint and trapezoidal rules. For these symmetric schemes of low order, it is well known that smoothing has a significant role in damping oscillatory errors, increasing stability for local extrapolations, and restoring classical asymptotic expansions. In addition to these difficulties, symmetric schemes of high order also suffer from the phenomenon of order reduction for stiff problems, and therefore some kind of smoothing is necessary too.

In this talk we consider generalizations of smoothing formulae for arbitrary symmetric Runge-Kutta methods that preserve the h^2 -error expansion and has the attractive feature of cheap implementation.

Numerical solutions to Nekrasov's equation

G. A. Chandler, University of Queensland, Australia and University of Bath.

Nekrasov's integral equation

$$\phi_\mu(s) = \frac{1}{3\pi} \int_{-\pi}^{\pi} \log \left(\frac{1}{|2 \sin((s-\sigma)/2)|} \right) \frac{\sin \phi_\mu(\sigma)}{\frac{1}{\mu} + \int_0^\mu \sin \phi_\mu} d\sigma,$$

gives the slope, $\phi_\mu(\sigma)$, of a steady wave on the surface of an infinitely deep ocean modelled by potential flow. Here $\phi_\mu(s) \geq 0$, for $s \geq 0$, and the parameter μ is large, say $\mu = 10^{20}$. It is known that as $\mu \rightarrow \infty$, $\max\{\phi_\mu(s) : s \geq 0\} \rightarrow 30.37^\circ$ although $\max\{\phi_\infty(s) : s \geq 0\} = 30^\circ$. This is the result of Gibb's phenomenon in a small boundary layer of width about $70/\mu$ near the crest $s = 0$.

We compute solutions to Nekrasov's equation that are accurate enough to resolve these oscillations. The integral equation is written as a Cauchy principal value operator, which is discretized by a simple singularity subtraction and a high order Gauss rule. Acute grading of the mesh gives sufficiently accurate solutions in the boundary layer to resolve oscillations with amplitudes about 0.8×10^{-70} .

The Numerical Treatment of Wiener-Hopf and Related Integral Equations with an Application in Outdoor Sound Propagation

Simon Chandler-Wilde, University of Bradford.

The paper considers second kind equations of the form $x(s) = y(s) + \int_{-\infty}^{+\infty} \kappa(s-t)z(t)x(t)dt$ abbreviated $x = y + K_z x$ in which x is the solution to be determined and the (known) factor z is bounded but otherwise arbitrary. Wiener-Hopf equations are included as the special case $z(t) = 1, t > 0, = 0, t < 0$. Existence-uniqueness is first considered: conditions on a set $W \subset L_{\infty}(\mathbb{R})$ are obtained such that a generalized Fredholm alternative is valid: if W satisfied these conditions and $I - K_z$ is injective for each $z \in W$ then $I - K_z$ is invertible for each $z \in W$ and the operators $(I - K_z)^{-1}$ are uniformly bounded. As a special case some classical results relating to Wiener-Hopf operators are reproduced. A finite section version of the above equation (with the range of integration reduced to $[-a, a]$) and projection methods for its solution are considered. Uniform stability and convergence results for the projection methods are obtained.

The numerical treatment, using a piecewise linear collocation method, of a boundary integral equation of the above type, which models outdoor sound propagation over inhomogeneous level terrain, illustrates the application of the results developed.

On a finite element method for 2D Semiconductor Diffusion Process Simulation

K. Chen, M. J. Baines and P. K. Sweby, University of Reading.

A new numerical technique for solving the Process Modelling diffusion equations has been proposed for the COMPOSITE simulation program. The spatial discretization, known as the ASWR method, is due to Svoboda and is a Petrov-Galerkin finite element method using quadratic B-splines. Time stepping is carried out using a three-level predictor corrector method. Here we report on the results of the stability and accuracy analysis of the method and on an alternative strategy of time step control. Numerical experiments on some full simulation problems have been carried out and results using the ASWR code are presented.

Recent Developments in the Application of Infinite Elements to Wave Diffraction

P.J. Clark, Newcastle University.

The solution of Helmholtz equation in two-dimensions has important applications in modelling water wave diffraction from marine structures. There have been two recent developments in the application of 'infinite' elements to the finite element solution of two-dimensional diffraction problems: mapped wave elements and mapped envelope elements. These elements are a little more complicated to calculate than finite elements of similar type but yield accurate solutions. The distinguishing feature of these elements is the form of test function used in the weighted residual equation. The mapped wave element yields a symmetric element matrix, and satisfies Sommerfeld's radiation condition implicitly, but is computed using a sophisticated product integration rule. On the other hand the mapped envelope element can be evaluated using Gauss-Legendre quadrature, but requires an explicitly formulated Sommerfeld radiation condition which produces an unsymmetric element matrix. The formulation of these elements is described and results are compared with f.e. solutions based on the cylindrical dampers of Bayliss and Turkel. Of particular interest is the use of these elements in high-frequency wave diffraction. Results are given for diffraction from an ellipse, a screen, and a semi-infinite wedge.

Analysis of a Family of Chebyshev Methods for $y'' = f(x, y)$

John P. Coleman and Andrew S. Booth, University of Durham.

Methods proposed by Panovsky and Richardson [J. Comp. Appl. Math., 23(1988)35-51] are interpreted as a family of symmetric two-step hybrid methods. Each method is based on a polynomial interpolant of degree n for y'' , for which the nodes are determined by the extrema of the Chebyshev polynomial of degree n . It is shown that the order of accuracy is $n + 1$ for n odd and $n + 2$ for even n , and expressions for the error constants are given. The stability properties of each method are determined by the roots of a quadratic equation $\lambda^2 - 2\alpha_n\lambda + 1 = 0$ where $\alpha_n(\nu^2)$ is a rational approximation for $\cos \nu$. The intervals of periodicity, which are also the intervals of absolute stability, are tabulated for $n \leq 10$. Numerical examples provide comparison with other methods.

Cubpack: A Suite of Codes for Numerical More-dimensional Integration

Ronald Cools, (Katholieke Universiteit Leuven, Belgium) and Ann Haegemans.

Until now the world of numerical more-dimensional adaptive integration consists of several routines which essentially do the same job in a somewhat different way: they all use the same global adaptive algorithm but use a different integration formula, a different error estimator, a different sorting algorithm and/or a different strategy for dividing the subregion(s) with the largest error. However changing one of the basic components leads to a totally different program. Someone having a new idea or a new cubature formula cannot use the existing routines and adapt them easily but has to start from scratch.

The basis of CUBPACK is a framework where changing one of the elements (the integration formula, the error estimation, the division strategy, ..) is done as easily as taking a cloth off a hatstand and hanging a new one on it. Therefore an object oriented and modular approach is essential. In this talk we will first explain the concept of the data-structure that is an essential starting point for the construction of CUBPACK. This data structure can be initialized by the user in an interactive way. We implemented this structure in FORTRAN 77 where we have to manage it with linear arrays.

Once this framework is set up we can do experiments on different strategies (classically a region is divided in 2 or 2^n regions but other scenarios are possible), different integration rules and different error estimators. All existing routines (without extrapolation) can be simulated with this project and combinations of elements can be made.

Decoupled fixed point and Newton schemes for the nonlinear systems arising in semiconductor modelling

Robert K Coomer and Ivan G. Graham, University of Bath.

In this talk we describe the numerical solution of the drift-diffusion equations in semiconductor device modelling. These are a coupled system of three nonlinear elliptic partial differential equations describing the electrostatic potential and the concentration of holes and electrons in a device. Discretizations are defined by the piecewise linear finite element method. Here we discuss the performance of several iterative decoupling strategies for solving the resultant nonlinear systems. We describe the theory of the fixed point (or Gummel) method, which converges linearly for small enough applied voltages. We also explain the mechanism whereby the decoupled Newton method converges quadratically in such voltage regimes. Both methods diverge unless the starting point of the iteration is sufficiently accurate. A continuation strategy for computing solutions for a sequence of voltages is described, and numerical results for the diode are given.

A Modified Numerov Integration Method for General Second Order Initial Value Problems
M. Van Daele (University of Gent), H. De Meyer and G. Vanden Berghe

We present a finite difference method for the general second order non-linear differential equation $y'' = f(t, y, y')$ subject to the initial conditions $y(t_0) = y_0$. This method is based on mixed interpolation of the form $f_n(x) = a \cos kx + b \sin kx + \sum_{i=0}^{n-2} c_i x^i$ in which the $n+1$ coefficients $a, b, c_0, c_1, \dots, c_{n-2}$ are determined by the conditions $f_n(x) = f(x)$ in $n+1$ equidistant points $x_j = x_0 + jk, j = 0, 1, \dots, n$ and where k is a free parameter. This free parameter makes it possible to construct a modified (implicit) Numerov method for which the accuracy is raised from sixth to eighth order in h . Using the same technique we have also established an explicit sixth-order integration-scheme. Both of these methods will be illustrated numerically on several examples.

Numerical solution of uncertain matrix equations with correlated entries, arising from modelling steady-state flow problems through heterogeneous porous structures
Mark Dainton, University of Reading.

A method for approximating the solution of a steady-state flow equation, with one parameter containing a correlated uncertainty is developed.

D'arcy's equation for two-dimensional steady-state flow through a porous medium with uncertain spatially variable permeability is considered. Because of obvious physical considerations, the variation in the permeability must be correlated in a spatial sense; quantitatively, this takes the form of a spatial correlation function that may or may not be isotropic.

The variation in the permeability is treated as a perturbation about some mean value, which may or may not be a spatially varying function. A discretization is performed: which results in a matrix equation, to be solved, where the elements of the matrix contain correlated statistical uncertainties, related to the permeability. A numerical perturbation series is then formed, and retaining terms up to second order allows the correlation function to be invoked to give mean values of the solution to the numerical approximation of the problem.

Instability in the approximation of the electric field integral equation
P. J. Davies, University of Dundee.

We discuss the stability of a time-marching finite difference approximation to the electric field integral equation which is used to solve the transient scattering problem for electromagnetic waves. A full stability analysis of the discretised scheme reveals the possibility of exponential growth in high spatial frequencies in the solution of the integral equation for the vector potential. We present some analytic and numerical results which demonstrate that this instability appears to be present for a wide range of values of the time/space mesh ratio, even for those values within the limits imposed by a standard CFL-type condition. We also indicate some possible ways of overcoming this problem.

A New Finite-difference Approach to Convection-dominated Flows with Application to Acoustic and Thermo-convection
Sanford Davis, NASA Ames Research Center, USA.

A series of compact, high-fidelity algorithms were developed for the first-order scalar convective wave equations. In this paper, the technique is expanded to a general system of nonautonomous matrix partial differential equations (Mpde's) representing the "locally

linearized" Navier-Stokes equations. These Mpde's are solved using a new space-time discretization for vector equations with matrix coefficients. With three spatial grid points and two time levels the method is formally fourth-order accurate for constant matrix coefficients. The deviation from fourth-order accuracy for this 3-point stencil depends on the smoothness of the coefficients. The approach used to develop the algorithm is based on phase dominance. This is precisely the criteria used to justify the asymptotic theory of wave propagation where a "fast" phase variable dominates a "slow" amplitude function.

Examples are presented from acoustics and thermo-convective flows to show that computational molecules developed from this "dispersion relation" approach capture a wide variety of physically plausible flows. In the first case it was able to accurately track an extremely phase-sensitive propagation problem. In the latter example, a complex flow exhibiting nonlinear instability is demonstrated. The thermo-convective Rayleigh-Benard problem serves as a model for the phenomenon of "global instability" which is commonly found in many technically important flows.

On resolvent conditions related to stability questions in the numerical solution of partial differential equations

J. L. M. van Dorsselaer, University of Leiden, The Netherlands.

Consider the so-called resolvent condition

$$\|(\zeta I - A)^{-1}\| \leq \frac{L}{d(\zeta, V)}, \quad \text{for all } \zeta \notin V.$$

Here V is a non-empty, closed subset of the complex plane. A is an $s \times s$ matrix ($s \geq 1$) and $\|\cdot\|$ is a norm on the vector space $\mathcal{C}^{s,s}$. Further, L is a positive constant, $L \geq 1$ and $d(\zeta, V)$ is the distance between the complex number ζ and the set V .

This condition has been recently discussed by various authors (Di Lena and Trigiante(1989), Grigorieff(1989), Kreiss and Wu(1990,1991), Lenferink and Spijker(1989), Lubich and Nevanlinna(1990), Reddy and Trefethen(1990,1991)) in studying stability questions occurring in the numerical solution of partial differential equations. In this talk we give some properties of this condition and discuss some examples.

Block Lanczos techniques for accelerating the block Cimmino method.

I.S. Duff (Rutherford Appleton Laboratory), M. Arioli, D. Ruiz and M. Sadkane

We consider acceleration techniques for the Block Cimmino iterative method for the solution of the consistent system of linear algebraic equations $Ax = b$, where A is an $m \times n$ sparse matrix ($m \leq n$) and b is an m -vector.

In this block iterative method, we partition A in a row-oriented way

$$A = \begin{pmatrix} A^1 \\ \vdots \\ A^p \end{pmatrix} \quad 1 \leq p \leq m.$$

For general systems, we exploit algorithms which maximize the minimum element on the diagonal, and which reorder A to block tridiagonal form. In this way, we can identify a partitioning in which A^i will be structurally orthogonal to A^{i+2} ($i = 1, 2, \dots, p-2$). In this case, the spectrum of the iteration matrix of the Block Cimmino method lies strictly between 0 and 2, is symmetric around 1, and has many eigenvalues clustered

around 1. For iteration matrices which are not too ill-conditioned, the conjugate gradient algorithm is a good method for accelerating the convergence of the iterative scheme. For ill-conditioned problems with poor convergence, we use preconditioning techniques and obtain an iteration matrix whose spectrum still has the same characteristics as those described above, but which also has clusters at the ends of the spectrum. Furthermore, in some test examples, these techniques are convergent whereas the Conjugate Gradient method is not.

Optimal Parallel Finite Difference Algorithms

D.B. Duncan, Heriot-Watt University.

We derive a timing model for the parallel implementation of nearest neighbour, finite difference algorithms on distributed memory parallel computers such as Transputer arrays and Hypercubes. The algorithm we consider allows some control over the balance between communications and computation costs and our timing model predicts that the start-up costs for the communications routines play a significant part in determining the optimal balance. We verify the model predictions in experiments on two different parallel computers and in some realistic cases obtain dramatic improvements in performance using the optimal version of the algorithm.

Algorithms for L_p approximation

Hakan Ekblom, Lulea University, Sweden.

An over-determined system of equations can be solved by minimizing the L_p -norm of the residual vector. We will look at algorithms for the case $1 < p < 2$, where an embedding technique combined with extrapolation has shown to be quite efficient. This also gives a background to the new IMSL routine RLLP.

DQAINTE: An Algorithm for Adaptive Quadrature (Vector Function) over a Collection of Finite Intervals

Terje O. Espelid, University of Bergen, Norway.

A new one-dimensional general purpose algorithm for adaptive quadrature will be presented. This algorithm differs from the well known general purpose code DQAG (QUADPACK) with respect to a number of aspects: three different local rules are offered: Gauss, Lobatto or Gauss-Kronrod; error estimation design; subdivision strategy: a non-uniform 3-division is applied; choice of data-structure: a heap. In addition the initial integration problem may consist of a collection of intervals (one problem but many intervals), simultaneous integration of a vector function is allowed and finally the code is designed to take advantage of shared memory parallel computers.

A FORTRAN 77 implementation of the algorithm, DQAINTE, has been tested both with respect to efficiency and reliability and some test results will be presented.

A finite difference procedure for a class of free boundary value problems

B Fornberg, Exxon Research, USA.

Finite difference schemes lose accuracy when free boundaries cross over rectangular grids. For a class of second order equations, the leading error term at such boundaries can be eliminated by a simple correction strategy. The procedure works in any number of space dimensions and offers an alternative to (more costly and complicated) adaptive grid techniques.

Parallel Optimization Techniques for Optimal Heat Integrated Separation Sequence Generation

E S Fraga and K I M McKinnon, University of Edinburgh.

The generation of optimal heat integrated separation sequences is an important and basic task in chemical process design. The efficient generation of these sequences is crucial. Design packages, which generate many such sequences, must approach trivial response time in order to be useful to a design engineer. The use of parallel computers is one approach taken recently to reduce the time required to determine the optimal sequences. Finding the optimal sequence has often been achieved using standard optimization techniques for combinatorial problems, including linear and nonlinear integer programming programming methods or implicit enumeration methods using branch and bound and/or dynamic programming techniques. We wish to concentrate on the use of branch and bound and dynamic programming techniques and their implementation on multi-computers, such as the INMOS T800 Transputer.

We show that different algorithms perform well on different problems. The particular features of the search tree (eg. its width) for a given subproblem can be used to determine which method is most likely to be the best. The careful selection of method allows us to achieve reasonable efficiency in a variety of problems. Results from experiments run on a Transputer-based 12 node multi-computer are shown.

A Boundary Integral Equation Method for the Numerical Solution of a Nonlinear Boundary Value Problem

M. Ganesh, University of Bath.

This paper is concerned with the numerical solvability of a nonlinear boundary integral equation (BIE) obtained by a reformulation of a nonlinear boundary value problem for Laplace's equation. We use a variation of the Kumar and Sloan collocation-type method to compute the numerical solution of the nonlinear BIE.

Under certain smoothness assumptions on the functions appearing in the nonlinear boundary condition, we show that the collocation-type approximate equations have unique solutions and the approximate solutions converge to the actual solution of the nonlinear BIE. We also analyse the rate of this convergence. Apart from the computational advantage of our method over a recent work in this direction, we obtain better rate of convergence of the approximate solutions.

A supraconvergent finite-volume scheme for the convection-diffusion equation

Bosco García-Archilla, Universidad de Valladolid, Spain and John MacKenzie, Oxford University.

Nonuniform grids are a useful tool to deal with differential problems whose solutions can develop large gradients. However, the analysis on nonuniform meshes can be much more involved than that corresponding to uniform grids. An example of such problems is the idea of supraconvergence, where a finite difference scheme, on nonuniform meshes, has an order of convergence higher than its order of consistency.

In this paper we try to gain more insight into the supraconvergence phenomenon by analysing the supraconvergence of a finite-volume method for the convection-diffusion equation. On nonuniform meshes, the scheme is second order convergent while being only first order consistent.

We present numerical experiments backing our findings.

The numerical detection of Hopf bifurcations in large systems arising from discretisations of P.D.E.S

T.J. Garratt, University of Bath, A. Cliffe, AEA Technology and A. Spence University of Bath.

In the analysis of nonlinear systems arising from discretisations of p.d.e.s, it is often necessary to compute a number of important eigenvalues of a large sparse nonsymmetric matrix, A say. The eigenvalues of importance are those with smallest real part and can be used to determine stability of a branch of steady state solutions and detect Hopf bifurcations. Most problems are too large to handle by standard methods such as the QR algorithm and attention is focused on methods requiring only matrix-vector operations on A . Two such methods are subspace iteration and Arnoldi's method, but when applied directly to A these methods will almost certainly not converge to the desired eigenvalues. To overcome this problem the methods are applied to a transform of A , with the transformed matrix having a spectrum such that convergence to the desired eigenvalues is expected.

Numerical Computation of Multivariate Normal Probabilities

Alan Genz, Washington State University, USA

The problem of computing $\text{Prob}(x_1 < a_1, x_2 < a_2, \dots, x_n < a_n)$ for a multivariate normal distribution with covariance matrix C is considered. Two new algorithms are presented. These algorithms use transformations of the n -dimensional infinite integration region to produce finite region integrals which can be evaluated with globally adaptive numerical multiple integration software. Numerical results are reported and the new methods are compared with other existing methods.

Computation of Takens-Bogdanov Points by a Direct Characterization

W. Govaerts(Rijksuniversiteit Gent), E. Chu (Monash University, Australia) and A. Spence (University of Bath).

We propose a direct method for the computation of Takens-Bogdanov points in two-parameter systems of nonlinear equations. Generically these points are found as the intersections of curves of fold points with curves of Hopf bifurcations. Their existence and the knowledge of their location is essential for the qualitative and quantitative understanding of the solution manifold of the system of equations.

Our method is based on a direct expression of the Jordan structure of the Jacobian with respect to the state variables in the Takens-Bogdanov points.

Compared to other methods, this one has the following features: (1) it is simple and natural, being based on linear algebra concepts only; (2) it treats the two parameters in a symmetric way; (3) it does not lead to formally large systems; (4) the nondegeneracy condition can be expressed in terms of the problem data only, not in terms proper to the algorithm; (5) it fits in a unified approach of folds, Hopf bifurcations, Takens-Bogdanov points and matrix problems such as the computation of real and complex eigenvalues of matrices; and (6) it provides further scope for a treatment of symmetry-breaking bifurcations and higher-order singularities in many-parameter problems.

Analysis of numerical methods for Nekrasov's equation

I. G. Graham, University of Bath.

In this talk we describe the analysis of a quadrature method for computing numerical solutions of Nekrasov's integral equation. For certain parameter ranges the solution

possesses a narrow boundary layer, the accurate resolution of which requires computation with strongly graded meshes. For the continuous problem, a solution is known to exist, but there is no local uniqueness result. In this talk we use global existence results from positive operator theory to show that the discretised equation also possesses a solution. Then we use a weak compactness argument to show that, as the mesh is refined, a subsequence of numerical solutions converges to a solution of the continuous problem.

Extrapolation of a Sequence of Functions

P.R. Graves-Morris, University of Bradford

Aitken's Δ_2 formula is widely known, and used when it is believed that the convergence of an ordinary sequence is dominated by a single geometric component. Given a sequence $S_0, S_1, S_2, \dots$, the transformed sequence is

$$T_r := S_r - \frac{(\Delta S_r)^2}{\Delta^2 S_r} = S_{r+1} - \Delta S_r \Delta S_{r+1} / \Delta^2 S_r, \quad r = 0, 1, 2, \dots$$

Aitken's formula corresponds to the Pade approximant of type $[1/1]$ for the generating function of the given sequence. It also corresponds to one iterative step of the epsilon algorithm.

This formula can be generalised to apply to functions, and for reasons which are not yet fully understood, the precision obtained on example problems has exceeded that of Aitken's formula quite dramatically. New results for acceleration of convergence, eigenvalues, eigenvectors etc. obtained by Thukral and Graves-Morris for the integral equation

$$\phi(x) = 1 + \lambda \int_{-1}^1 K(x, y) \phi(y) dy$$

with

$$K(x, y) = \begin{cases} (x+1)(1-y)/8, & -1 \leq x \leq y \leq 1 \\ (1-x)(y+1)/8, & -1 \leq y \leq x \leq 1 \end{cases}$$

will be reported.

Approximate Methods for Volterra-Fredholm Integral Equations

Lechoslaw Hacia, Technical University of Poznan, Poland.

Particular cases of Volterra-Fredholm integral equations of the second kind arise in the mathematical modelling of the spatio-temporal development of an epidemic and in the problems of the heat conduction. Approximate solution of these equations is proposed by various methods - projection-iterative method, collocation-iterative method, projection method. Sufficient conditions for the convergence of the considered methods are given and error estimates are obtained. Numerical examples illustrate the methods presented.

Applications of Preconditioned CG to Singular or Ill-Posed Linear Equations

Martin Hanke, Universität Karlsruhe.

We consider the iterative solution of linear equations $Ax = b$. Here, A may be a singular matrix such that b need not lie within the range of A (the *singular case*), or A may just as well be a bounded operator between two Hilbert spaces with non-closed range (the *ill-posed case*).

In both cases, popular algorithms for computing approximations z of x aim to minimize the residual norm $\|b - Az\|$ while keeping some seminorm $\|Lz\|$ as small as possible at the same time.

Iterative algorithms for this problem are easy to derive via the normal equations as long as L is injective. Here, we show how to design appropriate iterative methods if L has a non-trivial null space. If L is (the discretization of) a linear differential operator, the resulting algorithms may be implemented efficiently. Moreover, using the *preconditioned conjugate gradient method*, the residual is minimal at each step with respect to the associated Krylov space.

Making waves II: a numerical continuation method for finding periodic solutions in a class of differential-difference equations

P. S. Hansen, Technical University of Denmark and D. F. Griffiths.

Semidiscretization by means of the method of lines applied to wave equations, such as the model $u_t + u u_x = 0$, gives rise to space-periodic differential-difference equations of the form $\dot{u}_j = f(S^j u)$, where S is a shift operator. Under certain circumstances such semi-discrete equations have solutions that may be thought of as travelling waves.

A numerical method is developed for finding such solutions, based on the observation that it is only necessary to solve for $1/N$ th of the period and over one grid interval (N denotes the number of grid points). This restricted system may be recast as a first-order boundary-value problem with shifted-periodic boundary conditions. This problem is reduced to a system of nonlinear algebraic equations by the use of a high degree Hermite spline.

An extension of the method allows for computation of the (linearised) return map in a neighbourhood of the solution and thus for a study of the stability of the solution. Finally it is shown how to obtain a projection from the N -dimensional solution space to three dimensions to obtain pictures that are closely analogous to the 3-dimensional case.

Backward Error and Condition of Structured Linear Systems

Desmond J. Higham (University of Dundee) and Nicholas J. Higham (University of Manchester).

Existing definitions of backward error and condition number for linear systems do not cater for structure in the coefficient matrix, except possibly for sparsity. We extend the definitions so that when the coefficient matrix has structure the perturbed matrix has this structure too. We show that when the structure comprises linear dependence on a set of parameters the structured componentwise backward error is given by the solution of minimal ∞ -norm to an underdetermined linear system; we also obtain an explicit expression for the condition number in this linear case. Applications to symmetric matrices, Toeplitz matrices and the least squares problem are discussed and illustrated through numerical examples.

Optimization by Direct Search in Matrix Computations

Nicholas J. Higham, University of Manchester.

A direct search method attempts to maximize a function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ using function values only. Many questions about the stability and accuracy of algorithms in matrix computations can be expressed in terms of the maximum value of some easily computable function f . For a variety of algorithms it is shown that direct search is capable of

revealing instability or poor performance, even when such failure is difficult to discover using theoretical analysis or numerical tests with random or non-random data. The direct search methods used are the method of alternating directions and the multi-directional search method of Torczon. The problems examined include the reliability of matrix condition number estimators, the size of the growth factor in Gaussian elimination, and the stability of Strassen's fast matrix inversion method.

Introduction to CONFPACK, a Numerical Conformal Mapping Package

David M. Hough, Coventry Polytechnic.

I shall briefly outline the methods which are currently implemented in the software package CONFPACK for the construction of approximations to conformal maps on simply-connected domains. These methods are based on the numerical solution of Symm's integral equation. They involve the adaptive construction of Jacobi weighted variable degree piecewise polynomial approximations to certain boundary density functions. Several examples will illustrate the effectiveness of the package.

Parallel Diagonal-implicit Iterated Runge-Kutta methods

P.J. van der Houwen, CWI, Amsterdam.

In this talk an analysis of iteration schemes that are suitable for solving Runge-Kutta correctors on parallel computers will be given. We discuss the number of iterations needed to achieve the same stability and stiff accuracy properties as possessed by the corrector. These results indicate that the iterated methods require more (sequential) computational effort per step than the BDF methods. However, the higher orders of accuracy and the better stability properties allows much larger integration steps than is possible by BDF-based codes. The performance of the iterated Runge-Kutta code and the BDF (LSODE) code is illustrated by a number of examples.

Spurious Solutions of Numerical Methods for initial value problems

A.R. Humphries, University of Bath, UK.

It is well known that some numerical methods for initial value problems admit spurious limit sets. Here the existence and behaviour of spurious solutions of Runge-Kutta, linear multistep and predictor-corrector methods are studied in the limit as $h \rightarrow 0$. In particular, it is shown that for ordinary differential equations defined by globally Lipschitz vector fields, spurious fixed points and period 2 solutions cannot exist for h arbitrarily small, whilst for locally Lipschitz vector fields spurious solutions may exist for h arbitrarily small, but must become unbounded as $h \rightarrow 0$. The existence of spurious solutions is also studied for vector fields merely assumed to be continuous, and it is shown that if spurious fixed points or period 2 solutions exist for h arbitrarily small, then as $h \rightarrow 0$ spurious solutions either converge to steady solutions of the underlying differential equation or diverge to infinity. An example is given, showing that bounded spurious solutions can exist for continuous problems with h arbitrarily small. Also a necessary condition for the bifurcation of spurious solutions from $h = 0$ is derived. To prove the above results for implicit Runge-Kutta methods, an additional assumption on the iteration scheme used to solve the nonlinear equations defining the method is needed; an example of a Runge-Kutta method which generates a bounded spurious solution for a smooth problem with h arbitrarily small is given, showing that this assumption is necessary. It is also shown that an Adams-Bashforth/Adams-Moulton predictor-corrector method in PC^m implementation can generate spurious fixed point solutions for any m .

Parallel Optimization Using Variants of the Conjugate Gradient Algorithm to Solve a Finite Element Problem in Non-Linear Elasticity

P.K. Jimack, University of Leeds.

In this paper we derive a very large, but structured, unconstrained optimization problem from the finite element discretization of a three-dimensional variational problem in non-linear elasticity. We then consider and contrast implementations of various parallel solution algorithms, based upon the classical conjugate gradient method of Fletcher and Reeves. Finally, the relative efficiency of these approaches is demonstrated by showing computations performed on different numbers of transputers.

Iterated Defect Correction Methods for Nonlinear Differential Algebraic Equation of Index One

Bülent Karasözen, Middle East Technical University, Turkey.

This paper deals with the application of the iterated defect correction technique to differential-algebraic equations (DAE's) of index one in semi-explicit form. The convergence behavior of the defect corrections based on the linearly implicit Euler method is studied using the perturbed asymptotic expansions of the global error. At each defect correction step the order of convergence of numerical solutions is increased by one and the maximal attainable convergence order is limited by the degree of the interpolating polynomials. These theoretically predicted convergence results are confirmed on various test examples taken from linearly time varying and nonlinear index one DAE's. The results are also compared with those obtained by the extrapolation method. A code based on step size and order control is also developed and applied to some technical examples.

Some generalizations of wavelets: an algebraic approach

Jaroslav Kautsky, Flinders University, Australia

Wavelets are discussed explicitly, or in various disguises, in a wide range of literature on signal and image processing. Their mathematical foundation has been firmed in the language of functional analysis through works of Meyer, Daubechies, Mallat and others. Our aim is to give an algebraic exposition of wavelets. After all, in any application involving computer implementation (including those of signal and image processing) we finish working with finite sequences of values and performing mostly linear operations with them.

In this talk, the wavelets are viewed as linear algebraic transforms given by banded orthogonal matrices which can be built up from small matrix blocks satisfying certain conditions. We formulate the desirable properties of wavelets - orthogonality for reconstruction and regularity for concentration of information - in algebraic terms. A generalization of the finite support Daubechies wavelets is discussed and some special cases allowing more rapid signal reduction derived.

A Parallel L-stable Splitting Method for Multidimensional Parabolic Equations

A.Q.M. Khaliq, (Western Illinois University, USA) and D.A. Voss

A splitting method is constructed for multidimensional parabolic equations, which is second order accurate in space and time. For the semidiscretized PDE, the numerical solution is sought by employing rational approximations to the matrix exponential function. A novel rational approximation is developed which is L-acceptable and possesses real distinct poles. L-acceptability is a favorable property for PDEs with non-smooth

initial data. Parallelization is achieved by using a partial fraction technique and solving the resulting systems of linear equations on processors operating concurrently. The splitting method is implemented on the Alliant FX/8, a multiple instruction multiple data (MIMD) computer, utilizing four, and six processors for two and three dimensional problems respectively. Speedup and efficiency of the method is demonstrated on Alliant FX/8. Numerical results are shown for various problems from the literature and are compared with some well known splitting methods.

Fast Rectangular Matrix Multiplication and QR Decomposition

Philip A. Knight, University of Manchester.

In the last twenty-five years there has been much research into matrix multiplication methods that have an asymptotically smaller operation count than conventional multiplication. Most research has concentrated on square matrices, but in practical applications rectangular matrices are also important. For a general matrix multiplication method, we give an expression for the order of the operation count for the multiplication of rectangular matrices. We also derive an exact operation count for Strassen's method with rectangular matrices and determine the recursion threshold that minimises the operation count.

Fast multiplication methods can be exploited in calculating a QR decomposition of a matrix. We show that for Bischof and Van Loan's block method the order can be reduced through the use of a fast method with a carefully chosen block-size. We use our operation count for Strassen's method to determine when the fast algorithm achieves a lower operation count than the conventional one and show this occurs for matrices with dimensions in the hundreds. The fast orthogonal decomposition method is known to be numerically stable, and we confirm this with numerical tests.

On the Numerical Solution of the Heat Equation

J.F.B.M. Kraaijevanger, University of Leiden, The Netherlands.

In this talk we consider the method of lines applied to the one-dimensional heat equation on the interval $[0, 1]$ with zero boundary conditions.

It is well known that spatial discretization of this problem leads to the initial value problem

$$U'(t) = AU(t) \quad (t \geq 0), \quad U(0) = u_0,$$

where A is the $n \times n$ tridiagonal matrix $A = (\Delta x)^{-2} \cdot \text{tridiag}(1, -2, 1)$ and $\Delta x = (n+1)^{-1}$ is the grid spacing.

For the numerical integration we consider general time stepping procedures of the form

$$u_n = \phi(\Delta t \cdot A)u_{n-1} \quad (n = 1, 2, 3, \dots).$$

where ϕ is a rational function which approximates the exponential function, and $\Delta t > 0$ is the time step.

We discuss conditions on $\lambda = \Delta t/(\Delta x)^2$ which are necessary and sufficient for various stability properties of this procedure. We focus on the Euclidean norm and the maximum norm.

Derivatives of Eigenvalues and Eigenvectors of Matrix Functions

P. Lancaster, A. L. Andrew and K.-W. E. Chu, University of Calgary, Canada.

For an $n \times n$ matrix-valued function $L(\rho, \lambda)$, here ρ is a vector of independent parameters and λ is an eigenparameter, the eigenvalue-eigenvector problem has the form $L(\rho, \lambda(\rho))x(\rho) = 0$. Real or complex values for ρ and λ are admitted, and L is assumed to depend analytically on these variables. In particular, nonlinear dependence on λ is the main concern. On the assumption that the eigenvalue-eigenvector problem itself can be satisfactorily solved, a study is made of the derivatives, the effect of normalization strategies, and the solvability and condition of the bordered matrix equations arising naturally in this context. Implications for various classical eigenvalue problems $L(\rho, \lambda) = A(\rho) - \lambda I$ are clarified.

Stratified sequences of nested rules for fully adaptive quadrature

Dirk P Laurie, Potchefstroom University for Christian Higher Education, South Africa
Adaptive quadrature algorithms have the property that their behaviour is tailored to the integrand. Such algorithms may be adaptive in two ways.

- A nested sequence of quadrature rules, each more accurate than its predecessor, is applied. Examples of this approach are the methods of Romberg, Clenshaw and Curtis, and Patterson, as well as the various approaches based on variable transformation plus the trapezoidal rule. We call such algorithms *order adaptive* even though it is a misnomer for the transformation methods.
- A fixed quadrature rule is compounded by applying it on each subinterval of some partition of the quadrature interval. The partition is gradually built up by subdividing at each stage one of the current subintervals. Most of the QUADPACK algorithms are of this type. We call such algorithms *partition adaptive*.

It is conceivable that a quadrature algorithm could be order as well as partition adaptive. We call such an algorithm *fully adaptive*. At each stage, the selected subinterval is either subdivided, or a higher order quadrature rule is applied to it. Practical problems arise when a Patterson nested sequence is applied in a fully adaptive algorithm, because all quadrature points are reweighted, thus requiring storage of old function values for each subinterval under consideration. In this paper, we suggest the use of *stratified* nested sequences, characterized by the property that

$$Q_{k+1}f := c_k Q_k f + (1 - c_k) U_k f,$$

where Q_k is the nested rule at stage k , and U_k is a rule involving the new points only. No function values need be stored. We exhibit a new family of stratified nested rules constructed with $c_k = \frac{1}{2}$, with each rule interpolatory.

Solving Mixed Integer Nonlinear Programs by Quadratic Outer Approximation

S. Leyffer and R. Fletcher, University of Dundee.

Duran and Grossmann (1986) suggested an outer-approximation routine for solving a class of MINLPs by a finite sequence of relaxed MILP master programs and NLP subproblems. We generalize their idea by treating nonlinearities in the integer variables directly. Our approach is more natural, since we avoid adding extra variables or constraints to the problem. We give an example, for which the linear outer-approximation

routine of Duran and Grossmann exhibits the worst possible behaviour by visiting all feasible integer combinations. This has lead us to include a curvature term in the relaxed master programs resulting in an algorithm that solves MINLPs by a finite sequence of MIQP master programs and NLP subproblems. Our algorithm solves the example in two iterations.

A Petrov-Galerkin Formulation for Metal Forming Processes

Xin Kai Li, University of Leicester.

The focus of this paper is the modelling of the metal forming processes with the Eulerian reference frame. In this case, the modelling becomes a convection dominated problem. As is well documented, the standard Galerkin methods give rise to spurious oscillations when the problem is convection dominated. Hughes and Brooks have proposed a formulation which modifies the usual test functions by a perturbation dependent upon the flow lines and the derivative of the trial functions. This scheme is called the streamline upwind/Petrov-Galerkin (SUPG) method which allowed oscillations to be suppressed. In this paper, we apply this approach to the metal forming processes by modifying the test functions. Results of sample computational simulations of hot rolling are presented and clearly show that the Petrov-Galerkin method is more effective for solving nonlinear thermal elastic-plastic problems in the metal forming processes.

A method for creating practical parallel algorithms for large hyperbolic problems

Mark Lynch, Heriot-Watt Univeristy.

The development of parallel computers has made solving large multi-dimensional linear hyperbolic problems feasible. This computational environment gives rise to communication considerations in algorithm development, it is these considerations which tend to favour the explicit over the implicit algorithms.

For linear hyperbolic problems we apply Jacobi iteration to "good" implicit schemes to obtain new explicit schemes. In particular we show that the desirable stability, accuracy and isotropy properties of the implicit schemes can be captured with only a small number of iterations. We highlight a difficulty associated with the application of our procedure to some implicit schemes and give a method for overcoming it.

A dispersion correction method for FEM models of vibration

R. I. Mackie, University of Dundee.

Numerical models of waves and vibration modes produce errors. These errors are usually greater the higher the frequency of the wave. This means that very fine meshes have to be used to obtain accurate representations of the higher modes of vibration. This can result in prohibitively high computational costs. The nature of the errors can be investigated by studying the dispersion introduced by the numerical approximation. A correction scheme has been developed that uses this information and allows accurate answers to be recovered from initially inaccurate results, thus enabling good results to be obtained on coarse meshes. The method has been successfully applied to longitudinal vibration of bars and flural vibration of beams. The correction method can also be applied to the mode superposition method of modelling wave propagation.

Data Dependent Triangular Grid Generation
Andrew Malcolm, University of Reading.

Until recently, methods of triangulating a domain relied on geometrical constraints e.g. the position of the nodes on the interior of the region. However it is possible that for the interpolation of functions on the domain such geometrically generated triangulations can produce very poor representations of this underlying data. To improve the quality of the representations, methods will be presented which generate data dependent triangulations either by reconnecting the edges in the triangulation, by moving the nodes with a fixed connectivity or by generating the nodes and the triangles concurrently in a moving front procedure.

The Polar Decomposition

Roy Mathias, The College of William and Mary, USA.

Let A be an $n \times n$ matrix. The polar decomposition of A is $A = UP$, with U unitary and P positive semidefinite. If A is non-singular then U is unique and denoted $U(A)$. (P is always unique.) I will concentrate on the unitary factor. The positive definite factor is also of interest, especially because its eigenvalues are the singular values of A .

I will briefly survey

1. Applications of the polar decomposition
2. Inequalities involving the polar decomposition
3. Methods for computing the polar decomposition

and then present some new perturbation bounds for $U(A)$ and the inequalities for Hadamard products on which they depend.

Geometric Methods for Computing Invariant Manifolds

G. Moore, Imperial College.

Most methods for calculating invariant manifolds of differential equations follow, directly or indirectly, solution trajectories on the manifold. We consider the manifold as a geometric object and wish to compute it independent of the dynamics of the underlying differential equation. Applications of the basic idea to periodic solutions, connecting orbit pairs and invariant tori will be presented.

Order Barriers and Characterizations of Continuous Mono-Implicit Runge-Kutta Schemes

Paul Muir and Bryn Owren, University of Toronto

The mono-implicit Runge-Kutta schemes, a subset of the family of implicit Runge-Kutta schemes, were originally proposed for the numerical solution of initial value ordinary differential equations more than fifteen years ago. During the last decade, there has been considerable investigation of the use of these schemes in the numerical solution of boundary value ODE problems, where their efficient implementation suggests that they may provide a worthwhile alternative to the widely used collocation schemes. In fact, recent work in this area has seen the development and testing of software packages for boundary value ODE's based on these schemes. Unfortunately, these schemes lead to algorithms which provide only a discrete solution approximation at a set of mesh points over the

problem interval, while the collocation schemes provide a natural continuous solution approximation. An approach for the construction of a continuous solution approximation based on the mono-implicit Runge-Kutta schemes is suggested by recent work in the area of continuous extensions for explicit Runge-Kutta schemes for initial value ODE's. In this talk, we describe our work in the investigation of continuous versions of the mono-implicit Runge-Kutta schemes: (i) we establish lower bounds on the number of stages needed to derive continuous mono-implicit Runge-Kutta schemes of orders 1 through 6, (ii) we provide characterizations of all such schemes having an minimal number of stages for each of these orders, and (iii) we present particular examples of interpolants for each of these orders that have been implemented within a software package based on defect control for the numerical solution of boundary value ODE's.

QMR: A Quasi-Minimal Residual Method for Non-Hermitian Linear Systems

Noel M. Nachtigal and Roland W. Freund, Massachusetts Institute of Technology, U.S.A.

The biconjugate gradient (BCG) method is the natural generalization of the classical conjugate gradient algorithm for Hermitian positive definite matrices to general non-Hermitian linear systems. Unfortunately, the original BCG algorithm is susceptible to possible breakdowns and numerical instabilities. In this paper, we present a novel BCG-like approach, the quasi-minimal residual (QMR) method, which overcomes the problems of BCG. An implementation of QMR based on a look-ahead version of the nonsymmetric Lanczos algorithm is proposed. It is shown how BCG iterates can be recovered stably from the QMR process. Some further properties of the QMR approach are given and an error bound is presented. Finally, numerical examples are reported.

Numerical computation of an analytic singular value decomposition of a matrix valued function

N.K. Nichols, A. Bunse-Gerstner, R. Byers and V. Mehrmann, University of Reading.

This paper extends the singular value decomposition to a path of matrices $E(t)$. An analytic SVD of a path $E(t)$ is an analytic path of factorizations $E(t) = X(t)S(t)Y(t)'$ where $X(t)$ and $Y(t)$ are orthogonal and $S(t)$ is diagonal. To maintain differentiability the diagonal entries of $S(t)$ are allowed to be either positive or negative and to appear in any order. This paper investigates existence and uniqueness of analytic SVD's and develops an algorithm for computing them. We show that a real analytic path $E(t)$ always admits a real analytic SVD and that a full-rank, smooth path $E(t)$ with distinct singular values admits a smooth SVD. We derive a differential equation for the left singular factor and use it to develop a numerical method for tracking an analytic SVD. Convergence of the method is established.

Chebyshev pseudo-spectral methods for the KdV equation

F N Nouri, University of Annaba, Algeria

Chebyshev pseudo-spectral methods are used to approximate the Korteweg-de Vries equation. The methods differ in their treatment of the boundary conditions and are compared for computational efficiency using the one- and two-soliton test problems. The effect of time-filtering is also studied.

Non-negative Area Matching "Histosplines", a Local Approach

Gerhard Opfer, University of Hamburg, Germany.

A spline s defined on a grid $a = t_1 < t_2 < \dots < t_n = b$ is called a histospline if it matches prescribed areas a_j between neighbouring nodes, i.e., if $\int_{t_j}^{t_{j+1}} s(t) dt = a_j, j = 1, 2, \dots, n-1$. The terminology histospline and histopolation as well seems to be due to the Dresden school around J.W. Schmidt, cf. J.W. Schmidt & W. Heß [Hamburger Beiträge zur Angewandten Mathematik, A, Preprint 41, 1991, 15p.]. It is reasonable to require non-negativity of the spline if the given data are correspondingly non-negative. We investigate the local behaviour between neighbouring nodes. A precise knowledge of the local behaviour considerably simplifies the construction of a (global) non-negative spline on the whole grid.

Rosenbrock Methods for Partial Differential Equations

A. Ostermann, University of Innsbruck, Austria.

The aim of the talk is to study the order of convergence for Rosenbrock methods when applied to linear parabolic differential equations

$$u_t(x, t) = L(x, \partial) u(x, t) + f(x, t)$$

with appropriate initial and boundary conditions. Let p denote the classical order of the Rosenbrock method and let

$$\bar{\nu} = \sup\{\nu \in \mathbf{R} \mid f^{(j)}(\cdot, t) \in D(L^\nu), 0 \leq j \leq p\}$$

where $D(\cdot)$ is the domain of an operator. For example, for the one dimensional Laplace equation in $(0, 1) \times (0, T)$ with homogeneous Dirichlet boundary conditions and with $f(0, t) \cdot f(1, t) \neq 0$ one has $\bar{\nu} = 1/4$ in the space of square-integrable functions.

Our main result is: Under weak assumptions (i.e. $A(\alpha)$ -stability), the Rosenbrock method applied to the above equation is convergent of order

$$r = \min(p, q + 2 + \bar{\nu}).$$

Note that we have $q = 1$ unless the method fulfills supplementary order conditions (which will be discussed). Since typical values are $p = 4, q = 1, \bar{\nu} = 1/4$ one often gets the fractional order of convergence $r = 3.25$. Numerical examples illustrate these theoretical results.

Using divergent iterations in high accuracy, high speed computations, part 2

P. W. Pedersen, Technical University of Denmark.

The numerical solution of a boundary integral formulation for the two-dimensional Helmholtz equation in a perturbed half-plane.

Andrew Peplow and Simon Chandler-Wilde, University of Bradford.

We discuss the numerical solution of a boundary integral equation formulation of the two-dimensional Helmholtz equation in a perturbed half-plane D with smooth boundary ∂D , D consisting of the union of the upper half-plane, U , and a finite region S in the lower half-plane. The integral equation formulation is a system of three coupled equations, the unknowns, the pressure on the boundary of S , and the pressure and its normal derivative

on the interface between S and U . An interesting feature of the analysis is that the region S has two cusps. We show first that the integral equation formulation has a unique solution at all wavenumbers. The numerical method, a simple boundary element method, is described, a partial error analysis given and some numerical results presented.

Construction of Smooth Surfaces by Piecewise Tensor Product Polynomials

A. R. M. Piaah, University of Dundee.

The aim of this paper is to construct surfaces with tangent plane continuity defined by tensor product polynomials over a mesh of rectangles, by subdividing the mesh and keeping the continuity conditions across mesh lines fixed. We consider the space of all functions on a simple quadrilateral mesh (S.Q.M.) whose restrictions to each face are certain polynomials and which satisfy the continuity conditions across the edges. We construct a basis of positive functions with small support which sum to 1 and are useful for the design of surfaces. We also show that the space is suitable for interpolating data at the midpoints of the faces of the S.Q.M.

Interval methods for degenerate linear programming

Frank Plab, Edinburgh Parallel Computing Centre.

We describe a simplex-like algorithm for Linear Programming which maintains reliability even for highly degenerate problems. The algorithm is based on a method of Fletcher which dualizes the problem when degeneracy occurs. The original method of Fletcher has a guarantee of termination, but although it works usually well in practice there is no guarantee that it terminates at the exact solution. As a remedy we use interval arithmetic to control the roundoff error so that we obtain guaranteed bounds for the solution, which are refined by an iterative process.

On Preconditioning for Finite Element Equations on Irregular Grids

Alison Ramage and **Andrew J. Wathen**, University of Bristol.

One efficient algorithm for solving Galerkin finite element equations is the preconditioned conjugate gradient method. A large number of preconditioning strategies have been proposed, many of which have attractive theoretical convergence estimates on two-dimensional regular grid problems. However, when using irregular grids different considerations may arise.

Developing rigorous theory for irregular problems has proved to be more difficult than in analogous regular cases and, as a result, many aspects of working with unstructured finite element grids are a lot less well understood. Here we present some theoretical results which apply to any finite element grid regardless of irregularity. These are useful in the analysis of various preconditioners for irregular finite element problems.

We also observe that the attractive features of some standard preconditioners in two dimensions may not be retained for three-dimensional problems so again the criteria for selecting a preconditioner may be different.

Parallel Power-of-Two FFTs on Hypercubes

R. Renaut, Arizona State University, U.S.A.

Theoretical analysis of ordered power-of-two Fast Fourier transforms(PO2FFT) demonstrates that the most efficient algorithms for hypercube architectures do not always use nearest-neighbour communication. An unordered parallel PO2FFT of length N

can be obtained with D nearest-neighbour interprocessor communications of packets of length $N/2^{D+1}$, on a D -dimensional hypercube. The ordered PO2FFT which uses nearest-neighbour communication requires, however, D interprocessor communications for $r/2 \geq D$ and $2D - \text{int}(r/2)$ interprocessor communications for $r/2 < D$, where $2^r = N$. In this paper we show that an ordered PO2FFT can also be obtained with just D interprocessor communications for any r if the restriction that all communications are distance one is removed. This new algorithm uses $\text{int}(r/2)$ distance one and $d - \text{int}(r/2)$ distance two interprocessor communications. Packets of size $N/2^{D+1}$ are transmitted in both of the ordered PO2FFT algorithms. Thus comparative efficiency depends on the transmission times for interprocessor communications over distance one and distance two. These times are very close on the Intel iPSC2 and iPSC2/860. The time complexity of both these algorithms will be discussed and compared. It is shown that the distance two algorithm. Furthermore, if the problem of contention for multiple-hop transmission is solved an ordered PO2FFT with multihop becomes a promising candidate on a hypercube.

On the Numerical Inversion of the Laplace Transform in Reproducing Kernel Hilbert Spaces

G. Rodriguez and S. Seatzu, Universita di Cagliari, Italy.

We consider the numerical inversion of the Laplace transform with equally spaced data, under the hypothesis that the behaviour of the solution is known at the boundaries. More precisely we study the solution of the following integral equation of the first kind with discrete data:

$$\int_0^\infty e^{-s_i t} f(t) dt = F_i, \quad i = 0, 1, \dots, m-1$$

where $s_i = s_0 + ih$ for $i = 0, 1, \dots, m-1$ and $s_0, h \in \mathbb{R}^+$.

In this work we propose to solve this problem using a numerical method based on the following three steps:

1. transformation of the initial problem into an equivalent finite moment problem;
2. solution of the new problem into three different reproducing kernel Hilbert spaces;
3. choice for each test function of "optimal" values of s_0 and h .

Moving Mesh Techniques for Solving One-Dimensional PDEs

R.D. Russell, and Y. Ren, Simon Fraser University, Canada.

We discuss various aspects of the moving mesh problem for the solution of partial differential equations in one space dimension. First, we show that methods based (explicitly or implicitly) upon an equidistribution principle are associated with the problem of solving a particular PDE in the new computational coordinate system. Implementation of a discrete version of equidistribution to compute a moving mesh corresponds to solving a weak form of the PDE. This allows us to investigate the stability of the equidistribution process and to interpret various well-known strategies. Finally, some numerical examples are given to demonstrate the robustness of some new moving mesh strategies developed using this new framework, and their competitiveness with the standard moving mesh techniques (notably the moving finite element method) is shown.

The effect of high order nonlinear diffusion in a discrete form of Fisher's equation.

S.W. Schoombie, University of the O.F.S., South Africa.

We consider a discrete version of the equation

$$\frac{\partial u}{\partial t} = \frac{1}{N+1} \frac{\partial^2}{\partial x^2} (u^{N+1}) + u(1-u),$$

where N takes on nonnegative integer values. We investigate the existence and stability of the real period two solution

$$U_j^n = a + (-1)^{j+n}b$$

for various values of k , r and N , and show that $N = 7$ is a bifurcation point. Up to this value the stability region of the fixed point $u = 1$ is surrounded by a region of stable period two solutions, with no such solutions coexisting with the fixed point. For higher values of N , however, this is no longer true. We point out some of the consequences from the point of view of numerical analysis.

The Sticky Syrup Problem

P.W. Sharp, Queen's University, Kingston, Canada

One dimensional problems in fluid-flow that involve the draining of a fluid down a wall, or the coating of a surface by a fluid, are often modelled by third-order ordinary differential equations of the form $y''' = f(x, y)$. We derive and investigate classes of explicit Runge-Kutta pairs that integrate these problems directly.

The aim of the talk is two-fold. First, to show that the direct pairs are significantly more efficient than, and just as reliable as, Runge-Kutta (RK) pairs applied to the equivalent first order problem. Second, to investigate how the wealth of knowledge for RK pairs can be applied to the direct pairs.

On the choice of basis functions in the finite element solution of the shallow water wave equations

S. T. Sigurdsson, University of Iceland.

In the solution of the shallow water wave equations by the Galerkin finite element method one commonly chooses quadratic basis functions for the velocity components along with linear basis functions for the water elevation in order to ensure stability. This choice can be based on an analysis similar to that of the Stokes equations and relates to the Babuska-Brezzi condition. However since the Laplacian of the velocity components does not enter into the shallow water wave equations we shall argue that an equally stable, and in some computational respects more flexible and attractive, alternative is to combine the linear basis functions for elevation with piecewise constant functions for the velocities. We present a weak formulation of the equations along with a related stability condition justifying this choice and discuss some of the computational advantages, including the treatment of the nonlinear convective terms.

Fast Iterative Techniques for Finite Element Solution of the Stokes Problem

D. J. Silvester, (UMIST and Stanford University, USA) and A. J. Wathen.

Having an efficient Stokes solver is an important requisite of many Navier-Stokes solution algorithms. Iterative solution of the Stokes system is relatively straightforward since the

system is symmetric—the only impediment to efficiency is the indefinite nature of the system. Conventional wisdom is to formulate and solve the system for the dual variable (the pressure). Using this approach, the conditioning of the resulting matrix system is independent of the grid (assuming that the mixed finite element method is sufficiently stable). The disadvantage of this strategy is that an inner-outer iteration process is invariably required, with the convergence of the outer iteration being very sensitive to the convergence tolerance at the inner level.

In this talk we discuss a more direct solution approach, the intention being to avoid a decoupling into primary and dual variables. We present a ‘general theory’ which quantifies the relationship between the eigen-structure of the Stokes matrix, and the stability of the underlying mixed approximation. Our theory shows that, using so called ‘stabilisation techniques’, fast iterative solution of the Stokes system can be achieved. In particular, the ‘stabilisation parameter’ introduced can be tuned, to achieve rates of convergence analogous to that of a Poisson solver on the same discretisation. We also analyse the performance of preconditioning strategies which fit in a natural way with the ‘local stabilisation process’ used, and discuss implementation issues on shared-memory and distributed-memory parallel processors.

Computation of Inertial Manifolds

D. M. Sloan, University of Strathclyde, R. D. Russell and M. R. Trummer, Simon Fraser University, BC, Canada

The theory of inertial manifolds provides a connection between certain nonlinear dissipative partial differential equations (PDEs) and low dimensional dynamical systems. The restriction of the flow of the PDE to the inertial manifold is given by a finite set of ordinary differential equations called an inertial form, which captures the long-time dynamical behaviour of the PDE. We investigate various aspects of the problem of computing inertial manifolds for dissipative PDEs. In particular, we propose methods which generalise previous ones and improve upon some of their limitations. The methods are illustrated using models based on the Kuramoto-Sivashinsky equation and the Cahn-Hilliard equation. Iterative techniques are investigated by examining their ability to describe the qualitative behaviour of the models as demonstrated in their bifurcation diagrams.

On a Conjecture by LeVeque and Trefethen Related to the Kreiss Matrix Theorem M.N. Spijker, University of Leiden, The Netherlands.

In the stability analysis of numerical methods one is often faced with the question whether given $N \times N$ matrices A have powers that are uniformly bounded. Therefore, consider the property

$$\|A^n\| \leq M_0 \text{ for } n = 1, 2, 3, \dots,$$

where $\|\cdot\|$ denotes the spectral norm, and M_0 a constant.

In the Kreiss matrix theorem the above property is related to the so-called resolvent condition on the matrices A . LeVeque and Trefethen (1984) proved that the ratio of M_0 and the constant in the resolvent condition can be bounded by $2eN$. They conjectured that this bound can be improved to eN .

In this talk the conjecture is argued to be true. The proof relies on a lemma which provides an upperbound for the arc length of the image of the unit circle in the complex plane under a rational function. This lemma is of independent interest.

Numerical wave propagation in an advection equation with a nonlinear source term

Andrew Stuart (University of Bath), D.F.Griffiths (University of Dundee) and H. C. Yee (NASA Ames).

The Cauchy and initial-boundary value problems are studied for a linear advection equation with a nonlinear source term. The source term is chosen to have two equilibrium states, one unstable and the other stable as solutions of the underlying characteristic equation. The true solutions exhibit travelling waves which propagate from one equilibrium to another. The speed of propagation is dependent on the rate of decay of the initial data at infinity. A class of monotone explicit finite-difference schemes are proposed and analysed; the schemes are upwind in space for the advection term with some freedom of choice for the evaluation of the nonlinear source term. Convergence of the schemes is demonstrated and the existence of numerical waves, mimicking the travelling waves in the underlying equation, is proved. The convergence of the numerical wave-speeds to the true wave-speeds is also established. The behaviour of the scheme is studied when the monotonicity criteria are violated due to stiff source terms, and oscillations and divergence are shown to occur. The behaviour is contrasted with a split-step scheme where the solution remains monotone and bounded but where incorrect speeds of propagation are observed as the stiffness of the problem increases.

Analysis of the Cell Vertex Finite Volume Method

M. Stynes and K.W. Morton, University of Oxford.

When the cell vertex finite volume method is applied to convection-diffusion problems in one dimension, a 4-point scheme is generated. We prove convergence of this scheme on general graded meshes, with respect to an energy norm. The error bounds obtained do not depend on Sobolev norms of the solution, and can be made small on suitably chosen meshes.

The result is extended to first-order hyperbolic problems in an arbitrary number of dimensions. We show how this extension facilitates the choice of those cell residuals which should be set equal to zero in the cell vertex method; in general, it has not previously been clear how this choice should be made.

Extraction of Car Resistance Coefficients from Coastdown Data

Adrian Swift, Massey University, New Zealand

This communication describes a recent project which required application of numerical techniques in a practical situation. Analysis of coastdown data is a useful tool for extraction of rolling resistance and aerodynamic drag coefficients of a car. Cenek and Shaw, from Central Laboratories, Works Consultancy Service, New Zealand, published velocity-time profiles incorporating continuous on-board anemometry and road slope measurement. The numerical and statistical techniques required for extraction of parameter values and their confidence limits from these profiles are discussed.

The vehicle rolling resistance F_R and aerodynamic drag F_D were assumed to have the respective forms at speed v :

$$F_R = a_0 + a_1 v^n, F_D = a_2 [V \cos \psi]^2$$

where a_0, a_1, a_2 are functions of relative vehicle speed V and yaw angle ψ . Optimal values of the related rolling resistance and drag coefficients for a given data set are found from a non-linear least-squares fitting procedure. In the case $n = 1$, confidence limits on the

coefficients were obtained, together with the sensitivity of the coefficients to variations in the input data. Workers in the area of road-load calculations assume $n = 2$ and the implication of this from the coastdown analysis point of view is also considered.

Numerical Solution of Differential/Algebraic Boundary Value Problems with Application to Detonation Modelling

R.M. Thomas, UMIST

The modelling of detonation often gives rise to a parameterised free boundary value problem containing differential and algebraic equations modelling chemical kinetics, fluid flow and conservation laws. We shall consider a simple model of unconfined detonation. This model problem is a singular index one differential/algebraic boundary value problem; that is, it has index one throughout the interval of integration except at the free boundary, where it has index two. We shall show that it is possible to reduce the index to one over the entire range of interest, including the free boundary, and it is also possible to write the problem in semi-explicit form. We shall consider the advantages and disadvantages of this new formulation.

Estimation of the Blow-up Parameters for a Class of Ordinary Differential Equations

Yves Tourigny and Michael Grinfeld, University of Bristol.

In recent years, blow-up phenomena have become a major topic in the theory of nonlinear evolution equations. One of the dominant themes of blow-up theory concerns the behaviour of the solution near the blow-up time. The unknown parameters which characterise this behaviour are referred to loosely as blow-up parameters.

In this talk, we address the problem of estimating numerically the blow-up parameters for a class of ordinary differential equations for which the solution admits a formal McLaurin expansion about the known initial value. For this class, the relevant framework is the theory of differential equations in the complex domain. For instance, the problem of estimating the blow-up time then reduces to finding the radius of convergence of the given power series. This is a classical problem which, thanks to the available symbolic packages such as MAPLE or REDUCE is now within the scope of automatic computations. Approximation procedures based on such ideas will be discussed with the help of specific examples and some preliminary convergence results will be presented.

The Structure of Jacobians in Spectral Methods for Nonlinear PDEs

M R Trummer, Simon Fraser University, Canada.

When solving nonlinear partial differential equations with periodic boundary conditions, one frequently uses spectral methods. Implicit time-stepping, the computation of steady-state solutions, or the approximation of inertial manifolds lead to nonlinear equations which can be solved by Newton's method. In this talk we describe the structure of the Jacobian matrix for typical nonlinearities, namely those involving products of the unknown function and its derivatives. The characterization is based on a matrix representation of the semigroup of bi-infinite sequences with the convolution operation.

On non-parametric constrained interpolation

K. Unsworth and B.H. Ong, University of Dundee.

This talk considers constrained interpolation for C^1 non-parametric piecewise rational cubic curves. That is, we consider curves which interpolate data points which lie entirely

on one side of a *given* constraint curve, and also interpolate the derivative which is given at each data point. The interpolating curves should also lie entirely on the same side of the constraint curve. Both straight lines and quadratic curves are considered as constraint curves.

The ideas that we use are based upon earlier work (joint with T.N.T. Goodman) which considers G^2 *parametric* piecewise rational cubic curves which interpolate given data and are constrained to lie entirely on one side of one or more straight lines.

Some New Families of Explicit Runge-Kutta Methods

J.H. Verner and P.W. Sharp, Queen's University, Canada.

Explicit Runge-Kutta formula pairs form a class of efficient algorithms for treating non-stiff systems of initial value problems in ordinary differential equations. Such formulas are derived by solving a set of nonlinear algebraic equations for the coefficients, and several different types are known. Among the most efficient pairs of orders 5 and 6 are those based on a FSAL design in which the approximation of order 6 may be propagated using eight stages, and the extra stage required to obtain the error estimating approximation of order 5 may be reused following any successful step.

In deriving such a family, Verner relied on the use of MAPLE to solve the algebraic equations. This presentation provides a more direct derivation of this family. This more natural formulation leads to the derivation of new higher-order pairs of the same design. It is then shown for each s that the family of $(s+1)$ -stage formula pairs of orders $(p-1)$ and p contains a proper sub-family of s -stage formula pairs of the same orders. For each pair of this new sub-family, the method of order p utilizes all s stages so that the method of order $p-1$ is properly imbedded. The new families are contrasted with others that are known, and some practical formula pairs of both types will be given in illustration.

Numerical Simulation of the Becker Döring Equations

C.H. Walshaw, Heriot-Watt University.

We consider a system of clusters of particles that can coagulate to form larger clusters or fragment into smaller ones. One model of this coagulation-fragmentation process is the Becker Döring equations:

$$\begin{aligned}\dot{c}_1(t) &= -J_1 - \sum_{r=1}^{n-1} J_r \\ \dot{c}_r(t) &= J_{r-1} - J_r \quad 1 < r < n \\ \dot{c}_n(t) &= J_{n-1}\end{aligned}$$

where c_r denotes the number of clusters of size r and

$$J_r = a_r c_r(t) c_1(t) - b_{r+1} c_{r+1}(t).$$

For certain choice of coefficients a_r, b_r and initial conditions $c(0)$ the system exhibits metastability, i.e. some of the solution components remain seemingly in (non-trivial) equilibrium for a very long time before decaying to their true equilibrium.

Numerical time-integration of the system clearly shows this metastability, however by its very nature direct simulation can be a painstaking process. Fortunately, the ODE solver can be parallelized reasonably efficiently and we give the results of some experiments

run on an array of transputers. Finally, we propose a numerical tool for calculating the metastable values of the components.

The eigenvalue spectra of banded Toeplitz and quasi-Toeplitz matrices

R. F. Warming and R. M. Beam, NASA Ames Research Center, USA.

Toeplitz matrices occur in many mathematical as well as scientific and engineering applications. In this paper we consider the eigenvalue spectra of banded Toeplitz and quasi-Toeplitz matrices. In particular we are interested in matrices of large but finite order and relatively small bandwidth. These are the types of matrices that appear in the investigation of stability and convergence of finite-difference approximations to differential equations. The quasi-Toeplitz matrices are the result of non-Dirichlet boundary conditions for the finite-difference approximations. First we show that an asymptotic (large matrix order) approach partitions the eigenvalue spectrum of a quasi-Toeplitz matrix into two parts. One part is independent of the boundary conditions and the spectrum is the same as for a pure Toeplitz matrix. The other part depends on the *uncoupled* boundary conditions and the Toeplitz coefficients. Next we present algorithms for both parts of the spectrum. Examples are used to demonstrate the utility of the algorithms, to present some of the interesting spectra, and to point out some of the difficulties encountered when conventional matrix eigenvalue routines are employed. Finally we consider the Toeplitz generalised eigenvalue problem which occurs, for example, in the stability analysis of Pade finite-difference approximations to differential equations.

Variational Bounds on the Entries of the Inverse of a Matrix

A.J. Wathen, (University of Bristol) and P.D. Robinson, University of Michigan, Ann Arbor.

Variational principles arise in many areas of applied mathematics and mechanics where equilibria are characterised by minimum energy. In Numerical Analysis, discrete analogues are used, for example, in deriving and analysing finite element methods for equilibrium problems. The classical Rayleigh Quotient is a useful theoretical and practical tool in Numerical Linear Algebra, but other variational principles are not common in this area.

In this talk we will describe the use of variational and bivariational techniques to derive bounds on the entries of the inverse of a real matrix. (A variational bound is an inequality involving real functionals which is valid for any choice of a single trial vector. A bivariational bound is similar, but involves two independently varying trial vectors.) Our results are based on generalisations of the Rayleigh functional and give bounds on the individual entries of the matrix inverse in terms of simple combinations of the entries of the original matrix.

We give results for symmetric positive definite matrices, non-singular symmetric indefinite matrices and for general real non-symmetric, non-singular matrices.

Bounds on the entries of the inverse of a matrix are useful in many situations where a priori bounding estimates for linear system solutions are required.

Minimizing a smooth function plus the sum of the k largest eigenvalues of a symmetric matrix

G A Watson, University of Dundee.

The problem is considered of minimizing an expression consisting of the sum of a smooth function and the k largest eigenvalues of a symmetric matrix, where the smooth function,

and the elements of the matrix depend on a finite number of free parameters. In general, the eigenvalue sum is not differentiable, and it is shown how the problem can be solved efficiently using a modification of techniques developed by Overton for minimizing the largest eigenvalue of a symmetric matrix. The method uses a trust region to give a global convergence property, and is also usually locally convergent at a second order rate. Numerical results are given to illustrate the performance of the algorithm on some test problems.

Superconvergence of Recovered Gradients of Finite Element Approximations to Elliptic and Parabolic Problems

J.R. Whiteman, Brunel University.

Superconvergent error estimates are derived for the recovered gradients of piecewise linear and piecewise quadratic finite element approximations to elliptic problems and systems. The dependence of the estimates on the regularity of the solutions is illustrated. These results are then extended to parabolic problems where the numerical approximations are derived with Galerkin in space/finite difference in time methods.

Best Chebyshev Approximation from Families of Ordinary Differential Equations

Jack Williams and Z. Kalogiratos, University of Manchester.

Within the framework of the Meinardus and Schwedt theory of nonlinear Chebyshev approximation we consider the approximation of functions and data by approximants generated from the solution of parameter dependent initial value problems in ordinary differential equations. Conditions for uniqueness and characterisation of best approximations are obtained in terms of properties of the differential equation. Some illustrative numerical examples of best approximations will be presented.

Parallel Algorithms for QR Decomposition on a Shared Memory Multiprocessor

K. Wright, University of Newcastle-upon-Tyne.

A variety of parallel implementations of algorithms for the QR decomposition of a matrix based on Givens rotations and Householder transformations are compared. The algorithms were devised for shared memory multiprocessors, and implemented on two bus-connected shared memory Encore Multimax computers, with different numbers of processors and different processor speeds. These implementations were then compared empirically. The programs were written initially in Pascal using the Encore multi-tasking library. To provide generality test runs used both long and short precision, and compilation with and without array bound checking. To provide further comparisons some of the algorithms were implemented in Encore Parallel Fortran (EPF), a Fortran77 extension including parallel constructs.

Although good speed up with both Givens and Householder algorithms were obtained, the results indicate one version of the Householder algorithm was significantly better than the other algorithms.

Tidal Barrage Optimal Control

Z.G. Xu and N.K. Nichols, University of Reading.

The optimal control problem in a tidal power generation scheme with two controls (sluices and turbines operating independently) is formulated. By applying Pontryagin's Maximum Principle the analytical forms of the optimal controllers can be derived for various

forms of the power function. In order to obtain the precise form of the solution, a numerical solution procedure is employed. It consists of a constrained optimisation algorithm for iteratively determining the optimal control functions, together with a finite difference scheme for solving the state and adjoint equations. The main aim of the numerical work is to find a suitable optimisation algorithm for the problem. For this purpose several gradient based optimisation algorithms, namely conjugate gradient (CG) and projected gradient (PG) algorithms, are investigated and the behaviour of the algorithms is examined. It is shown that the CG algorithm is the most efficient for bang-bang type controls, while the PG algorithm is the most efficient for controls with interior solutions.

Parallel orthomin for general sparse matrices

Zahari Zlatev, Danish Environmental Research Institute, Denmark.

Consider the system of linear algebraic equations $Ax = b$ where A is an $n \times n$ real matrix with $\text{rank}(A) = n$. Assume that A is a general sparse matrix; i.e. (i) A has no special property such as symmetry or positive definiteness, (ii) A has no special structure such as bandedness and (iii) A is large and contains many zeros. Assume also that an incomplete LU factorization can be obtained by using parallel pivots and by dropping "small" non-zero elements. Then the incomplete LU factorization is used as a preconditioner in an orthomin algorithm. An important property of the method is that the number of Krylov vectors used is not fixed in advance. The code starts with a prescribed number of Krylov vectors and increases it whenever the convergence is judged to be slow. Moreover, the algorithm is optimized for parallel computers with shared memory (such as the ALLIANT). Switching from dense matrix technique to sparse matrix technique is used to increase the efficiency. The stopping criteria are carefully chosen. The ideas applied in the development of the algorithm are illustrated by using many test matrices from the well-known Harwell-Boeing set.