

**13th BIENNIAL CONFERENCE
ON
NUMERICAL ANALYSIS**

**UNIVERSITY OF DUNDEE
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ABSTRACTS

**Section A: Invited Talks
Section B: Submitted Talks**

Section A: Abstracts of Invited Papers

Moving Finite Elements.

M. J. Baines, University of Reading, U.K.

Moving Finite Element methods solve time dependent PDE's using finite elements on moving grids. The grid velocity has to be generated in a suitable way, for example using equidistribution, mechanical analogies of the PDE itself. In the Moving Finite Element Method of Keith Miller the PDE is used in a natural extension of the usual semidiscrete fixed finite element procedure. It is shown that this procedure gives rise to an approximate Hamiltonian system implying that the nodal trajectories imitate the characteristics of the PDE. Surprisingly, the system of characteristic trajectories is obtained even when analytically the PDE does not warrant one. It is also shown that the approximation may be characterised geometrically through the use of a Legendre Transformation and an envelope construction. Indeed the numerical construction of any Legendre Transformation may be achieved by the techniques of the Moving Finite Element Method.

The analysis of the grid velocity throws light on the desirability of moving the nodes in this way. Illustrations are given for a range of problem areas.

Parallel multilevel preconditioners.

J. Bramble, J. Pasciak and J. Xu, Cornell University, USA.

A simple preconditioner based on multilevel decomposition of finite element spaces will be presented. This preconditioner is given as a sum whose terms are completely independent and thus may be computed in parallel. The resulting condition number of the preconditioned system is, in the worst case, on the order of the square of the number of levels k . For the usual finite element equations $k = \log 1/h$ where h is the fine mesh size. Applications are given to the usual finite element equations for second order elliptic problems as well as to meshes resulting from adaptive grid refinements. In contrast to the hierarchical basis preconditioner our construction is completely parallelizable and the condition number does not degrade for problems in higher dimensions.

The hunting of the SNARK, or Why the trapezoidal rule is algebraically stable

K. Burrage, University of Auckland, New Zealand.

*They sought it with thimbles, they sought it with care;
They pursued it with forks and hope;
They threatened its life with a railway-share;
They charmed it with smiles and soap.*

*They hunted till darkness came on, but they found
Not a button, or feather, or mark,
By which they could tell that they stood on the ground
Where the Baker had met with the Snark.*

*In the midst of the word he was trying to say,
In the midst of his laughter and glee,
He had softly and suddenly vanished away -
For the Snark was a Boojum you see.*

From the hunting of the Snark by Charles Dodgson.

Two important recent advances in the study of numerical methods for solving ordinary differential equations are the concepts of B-convergence and algebraic stability. There is a very close relationship between these but, unfortunately, they do not appear to be equivalent because of the example of the trapezoidal rule which is B-convergent but not algebraically stable when interpreted as a Runge-Kutta method. This has been the source of much puzzlement and even annoyance to many numerical analysts.

In this paper we show that this angst is unnecessary. The trapezoidal rule is algebraically stable if interpreted in the right way - as a Nordsieck rather than a Runge-Kutta method. We extend this approach and examine the algebraic stability of a general class of methods, known as multivalued methods and show that other apparent contradictions that arise when methods are interpreted as Runge-Kutta methods evaporate when they are looked at from a different and more appropriate viewpoint.

Quadratic Affine-Scaling Algorithms for Piecewise Linear Problems.

T. Coleman, and Y. Li, Cornell University, USA.

Recently Coleman and Li have shown how to solve linear L_1 problems with a global and (ultimately) quadratically convergent affine-scaling algorithm. In this talk we illustrate the practicality of the method and discuss implementation issues. Moreover, we will indicate how to adapt the underlying ideas to other piecewise linear problems such as the L_∞ problem.

Uniqueness Theorems for Stiff ODE Initial Value Problems.

P. Deufhard, Konrad-Zuse-Zentrum für Informationstechnik, Berlin, F.R. Germany.

Reliable numerical algorithms are, in one way or the other, appropriate implementations of uniqueness theorems of the underlying analytic problem. In non-stiff numerical integration, the associated uniqueness theorem for ODE initial value problems is the well-known *Picard-Lindelöf theorem* - which characterises the growth of the solution by means of the Lipschitz constant of the right-hand side of the ODE system. For stiff integration, this characterisation is known to be inappropriate, but an associated analytic uniqueness theorem in terms of a different characterisation seems to be missing - despite of the enormous amount of literature dealing with stiff integration. Such an analytic uniqueness theorem should then serve as a theoretical frame for investigations of *discretization methods* for stiff ODE systems. After some preliminary considerations two variants of the intended theorem are derived on the basis of affine invariant convergence theorems for *Newton's method* in function space. The emerging theoretical characterisation is then used to derive comparison theorems for *implicit* one-step methods. The new theory has an impact also on the implementation of stiff integrators. A brief review of numerical experiments with semi-explicit extrapolation integrators is included.

Towards Reliable Linear Programming.

R. Fletcher and J. A. J. Hall, University of Dundee.

Difficulties with simplex-like methods for linear programming occur when degeneracy and round-off errors interact to cause cycling or other instances of non-termination. This paper develops a method of Fletcher (*Linear Algebra and its Applications*, Vol 106, 149-183, 1988) which allows guaranteed termination under these circumstances. This method may truncate small numbers to zero in a near degenerate situation in order to obtain exact degeneracy, which is then treated accordingly.

In certain situations it has been observed that these truncations can cause significant changes to the solution of the LP problem. A strategy for avoiding these difficulties is described. The method is also extended to cover upper and lower bounds on all variables and constraints, and to allow the use of pseudo-constraints. A dense matrix production code has been developed, including the provision of warm and hot start facilities, etc.

A sparse matrix version of the code is now nearing completion. A simple-to-use scheme, requiring no provision for fill-in, is obtained by combining Tarjan's algorithm for block triangularization with Schur complement updates. A stable update for LU factors of the Schur complement, based on using the Fletcher-Matthews method, is described. Some numerical results on a standard large-scale test set are discussed.

Rapid Generation of Weights in Finite Difference Formulas.

Bengt Fornberg, Exxon Research and Engineering Co., USA.

We consider the problem of calculating the optimal weights in finite difference approximations of any order derivative, to any order of accuracy. In the special case of equispaced grids (and with the approximations desired at a grid point or half-way between grid points), there are very effective classical techniques available (less than 20 lines of code, costing only about 4 arithmetic operations per weight).

An equally short and efficient algorithm was recently discovered for the general case (i.e. for an arbitrarily spaced grid and with the approximations accurate at any fixed position, on or off a grid point). The anticipated applications of this algorithm include convenient generation of weights near boundaries, fast re-tabulating in cases of dynamically changing grids etc.

In the special case of interpolation (zero'th derivative), the new method turns out to be faster than (but mathematically equivalent to) the traditional implementations of Newton's interpolation formula (the algorithms by Aitken and Neville).

Boundary Integral Methods for Laplace's Equation.

I. Graham, University of Bath, U.K.

The direct boundary integral method is a popular fast method for solving homogeneous PDE's. For example, to solve Laplace's equation $\Delta\phi=0$ in a region Ω with boundary Γ , we employ Green's identity to represent ϕ in Ω as the difference of a single layer potential with distribution $\partial\phi/\partial n$ and a double layer potential with distribution ϕ . The boundary conditions then lead to (a system of) boundary integral equations for the unknown parts of the boundary data ($\phi|_{\Gamma}$, $\partial\phi/\partial n|_{\Gamma}$). In $\mathbb{R}^2$, when the boundary conditions are purely Neumann, second kind equations of the form

$$u(x) \pm \frac{1}{\pi} \int_{\Gamma} \frac{\partial}{\partial n(\xi)} \log\left(\frac{1}{|x-\xi|}\right) u(\xi) d\Gamma(\xi) = g(x), \quad x \in \Gamma, \quad (1)$$

arise, to be solved for the unknown $u|_{\Gamma}$. For pure Dirichlet problems, on the other hand, we have first kind equations of the form

$$\frac{1}{\pi} \int_{\Gamma} \log\left(\frac{1}{|x-\xi|}\right) u(\xi) d\Gamma(\xi) = g(x), \quad x \in \Gamma, \quad (2)$$

to be solved for $u=(\partial\phi/\partial n)|_{\Gamma}$. For mixed boundary conditions, a 2×2 system where one equation of each kind arises.

When Γ is smooth, the discretisation of (1), (2), and the iterative solution of the resulting linear system is now quite well understood. When Γ has corners (e.g. a polygon), the singularities induced in the integral operators and solutions make these questions

much more difficult. For (1), the quadrature method (standard for smooth problems) can be shown to converge optimally, provided it is modified slightly near corners. This modification then turns out to be essential for the convergence of multiple grid solution procedures for the resultant linear systems.

Much less is known about (2); for example, until very recently little progress had been made on understanding the very simple piecewise constant collocation method for (2) proposed by Symm in 1963. Some insight may be obtained by using a certain factorisation of the logarithmic integral operator in (2) to recast that equation as a (non standard) second kind equation. The difficulties arising in the (non standard) integral operator at the corners of the polygon are then very similar to those which arose in (1). Furthermore, Symm's collocation method may be thought of as a non-standard collocation method for this second kind equation. Using the theory of second kind equations, a (modified) collocation method for (2) may then be shown to converge. Moreover, the modification again provides the key to the fast multiple grid solution of the resultant linear systems.

This talk will survey joint work with other researchers on the above problems, with emphasis on the most recent results.

How Accurate is Gaussian Elimination?

N. J. Higham, Cornell University and University of Manchester.

Wilkinson put Gaussian elimination (GE) on a sound numerical footing in the 1960s when he showed that with partial pivoting the method is stable in the sense of yielding a small backward error. He also derived bounds proportional to the condition number $\kappa(A)$ for the forward error $\|x - \hat{x}\|$, where $\hat{x}$ is the computed solution to $Ax = b$. More recent work has furthered our understanding of GE, largely through the use of componentwise rather than normwise analysis. We survey what is known about the accuracy of GE in both the forward and backward error senses. Particular topics include: classes of matrix for which it is advantageous not to pivot; how to estimate or compute the backward error; iterative refinement in single precision; and how to compute efficiently a bound on the forward error.

Finite Element Methods for Compressible Flow.

C. Johnson, Chalmers University of Technology, Sweden.

We give an overview of some recent theoretical and computational results for the streamline diffusion finite element method applied to hyperbolic systems of conservation laws including the Euler equations for a compressible perfect gas. The streamline diffusion method is a general finite element method for hyperbolic problems combining high accuracy with good stability properties. Convergence is proved for general scalar conservation laws in several dimensions, also including boundary conditions on bounded domains, with piecewise polynomials of arbitrary order. For systems of conservation laws it is proved that if the finite element solutions converge to a limit, then the limit is a weak solution and satisfies all entropy inequalities associated with the given system. Numerical results obtained with an adaptive implementation of the method will be represented.

Knot Removal and Condition Numbers for B-Splines.

T. Lyche, University of Oslo, Norway.

Recently, Knut Morken and the author have developed a method for reducing the number of knots in a spline without perturbing the spline more than a given tolerance.

The number and location of the remaining knots are determined automatically. Knot removal has applications to the approximations of functions and data in the areas of computer aided geometric design, least squares with variable knots, constrained data fitting, smoothing of digitised curves, and detection of singularities at unknown locations. In the first part of the talk we will describe the knot removal method and give a new application to scattered data approximation.

The work on knot removal led us to reconsider the condition number problem for B-splines. We will look at this problem and some related condition numbers for discrete B-splines. Essentially, the problem is to determine the maximum size of the B-spline coefficients of a spline of unit norm. When the max norm is used the spline analog of the Chebyshev polynomials plays a prominent role for this problem. The extrema of this *equioscillating spline* turn out to be good candidates for interpolation points.

The Updating of Matrices of Conjugate Directions in Optimisation Algorithms.
M. J. D. Powell, University of Cambridge, U.K.

Many optimisation algorithms employ approximations to second derivative matrices of the objective function and they are usually stored in some factored form. In particular, if B is a positive definite second derivative approximation, then instead of storing B , we consider working with a matrix Z that satisfies $Z^T B Z = I$, so the columns of Z are conjugate with respect to B . There are many successful methods for updating B in order to include new second derivative information and there are analogous changes to Z . We take the view, however, that there is a family of changes to Z that are easy to apply and we ask whether some of these formulae correspond to standard updates of B . Thus we find a new implementation of a useful part of the well-known "Broyden linear family". Further, our methods for updating Z are particularly convenient for linearly constrained optimisation calculations, and we find too that some rescaling of columns of Z can give substantial reductions in the amount of work to solve several numerical test problems.

Eulerian-Lagrangian Localized Adjoint Methods for Advection-Dominated Problems.
T. F. Russell, University of Colorado at Denver, USA.

In collaboration with M. A. Celia, I. Herrera, and R. E. Ewing, we have recently formulated a space-time finite element methodology that builds on concepts of tracking advection-dominated flows (Eulerian-Lagrangian methods) and of optimal test functions (adjoint methods). With particular choices of elements and test functions, this yields the modified method of characteristics that we have investigated in the past. Advantages of the ELLAM formulation are a systematic treatment of boundary conditions, which have generally been handled in an ad hoc manner in Eulerian-Lagrangian methods, and a single scheme that covers the parabolic and hyperbolic cases of nonzero and zero diffusion. This talk will discuss the formulation, preliminary numerical results, and relationships to the H^{-1} -Galerkin method and streamline diffusion.

Some numerical aspects of Divide and Conquer Methods for Eigenvalue Problems
D.C. Sorensen, Argonne National Laboratory, USA.

An important new development in parallel algorithms for eigenvalue problems has been the advent of divide and conquer methods for both the symmetric eigenvalue problem and the singular value decomposition. These techniques have proven to be much faster than the standard algorithms even when run in serial mode. These techniques will be introduced and their numerical properties will be discussed.

Unfortunately, the Divide and Conquer technique can have difficulty in obtaining numerically orthogonal eigenvectors when there are extreme clusters of nearly equal eigenvalues. Two numerical techniques have been developed to overcome this difficulty. One involves an arrangement of the numerical calculations to assure extremely high accuracy in a function evaluation that is central to the calculation. The other involves a completely new technique for finding the zeros of this function in a way that directly involves the corresponding eigenvectors. Both techniques will compute eigenvectors that are accurate and numerically orthogonal to working precision even though there are several clusters of eigenvalues with a separation on the order of $10^{**}(-12)$ in a 64 bit finite precision arithmetic.

The Analysis and Numerical Analysis of Instabilities in Nonlinear Systems with Applications to the Navier-Stokes Equations.

A. Spence, University of Bath, U.K.

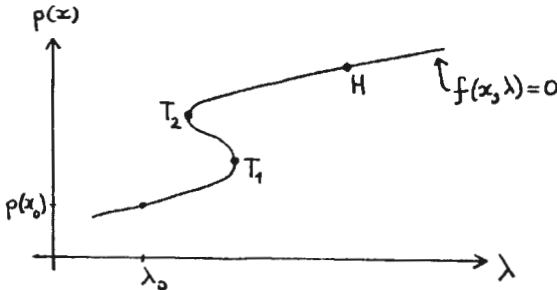
Many physical systems can be modelled as differential systems of the form

$$\dot{x} = f(x, \lambda), \quad x \in \mathbb{R}^n, \quad \lambda \in \mathbb{R} \quad (1)$$

with f nonlinear, and one of the most important problems in bifurcation theory is to identify the ways in which a steady state of (1) can lose stability as the parameter λ is varied. If (x_0, λ_0) is a steady state solution of (1), that is,

$$0 = f(x_0, \lambda_0) \quad (2)$$

then it is said to be *stable* if the eigenvalues of the Jacobian matrix $f_x^0 := [\frac{\partial f_i}{\partial x_j}(x_0, \lambda_0)]$ have negative real parts, and *unstable* if some of the eigenvalues have positive real parts. The steady state solutions satisfy $f(x, \lambda) = 0$ and we can use a numerical path following (continuation) code like AUTO or PITCON to help produce a bifurcation diagram, i.e. a plot of a functional of the solution, say $p(x)$, versus λ . A common type of solution path is given in the figure.



The points labelled T_1, T_2 are *Turning Points*, at which a *real* eigenvalue of f_x crosses the imaginary axis at zero, and the point labelled H is a *Hopf Bifurcation Point*, where a *complex conjugate pair* of eigenvalues of f_x crosses the imaginary axis. Depending on the spectrum of f_x the stability of a steady state solution may

change at both points. In the figure, for example, if (x_0, λ_0) is stable then it is possible that the parts of the path between T_1 and T_2 and to the right of H would be unstable.

In this talk we shall consider two cases when a system may lose stability. The first case arises in a two parameter system $\dot{x} = f(x, \lambda, \alpha)$ and occurs when a Hopf bifurcation point and a turning point coalesce (which is often called a *Takens-Bogdanov Point* or T-B point). When n in (1) is 'large', as is typically the case when considering discretizations of P.D.E's, then the detection of the presence of Hopf bifurcation points is a major computational problem and knowledge of the the solution structure near a T-B point can often help with this difficulty. To illustrate the theory we present some numerical results for a finite element discretization of the Navier-Stokes equations and these results can help explain the complicated stability exchange in experimentally observed 5-cell flows in the finite Taylor problem.

The second case arises in a one-parameter system like (1) but where f is equivariant with respect to an action of the group $O(2)$, that is,

$$\gamma f(x, \lambda) = f(\gamma x, \lambda), \quad \gamma \in O(2)$$

where $O(2)$ is the group generated by the rotations r_α , $\alpha \in [0, 2\pi]$, and a reflection s . In this case a steady state solution may lose stability to a *rotating wave solution*, which has the form $x(t) = r_{\omega t} x_0$, where x_0 is independent of time.

Once appropriate settings have been determined, it turns out that in both cases the analysis and numerical analysis is a straightforward application of reflectional symmetry-breaking bifurcation theory. Another unifying feature is that both cases correspond to steady solution points where f_x has a zero eigenvalue which is *geometrically* simple but *algebraically* double.

Computing the structured singular value, and some related problems.

G. A. Watson, University of Dundee, Scotland.

The concept of structured singular value was introduced by J C Doyle in 1982 as a tool for the analysis and synthesis of feedback systems with structured uncertainties. Mathematically, calculating this quantity involves finding the $n \times n$ block diagonal matrix Δ (with m blocks of specified sizes) of smallest spectral norm satisfying

$$\det(I + M\Delta) = 0,$$

where M is a given $n \times n$ matrix. One technique due to Doyle for solving this problem requires the (unconstrained) minimization of the spectral norm of a particular $n \times n$ matrix having $m-1$ parameters: some aspects of this kind of problem are considered. Another possible approach comes from the treatment of a general class of matrix perturbation problems, where it is required to find the smallest (in the sense of a given matrix norm) perturbation of a specified structure to produce rank-deficiency. A general class of algorithms for such problems is presented, and it is shown how this leads to the computation of the structured singular value through the solution of a minimax problem. This approach also permits the treatment of generalizations of the structured singular value problem.

Section B: Abstracts of Contributed Papers

Towards a Parallel, Commercial Oil Reservoir Simulator.

C. A. Addison, University of Liverpool, U.K.

The ECLIPSE 100 oil reservoir simulation package is one of the standard simulation packages used by oil companies working in the North Sea.

ECLIPSE has two computationally intense modules a) setting up a (possibly large and sparse) block tridiagonal matrix and subsequently b) solving a system of equations with this matrix using preconditioned ORTHOMIN iteration. The second of these modules is the more expensive of the two and was therefore the focus of a preliminary investigation into developing a parallel version of ECLIPSE.

The preconditioning used in ECLIPSE is inherently sequential. This means that a parallel version of ECLIPSE required a modified preconditioner. However, ECLIPSE is a commercial code and any parallel version would have to fit into an existing maintenance structure. Therefore the changes to the code had to be localised and not too extensive.

A block Jacobi preconditioner was used, with the existing preconditioner used within blocks. Such a preconditioner requires more iterations to converge, but because it is highly parallel, an overall speed-up was expected.

Experimentation to date has been limited, but results suggest that a parallel efficiency of between 1/3 and 1/2 should be expected on realistic problems within the linear solver.

A Criterion Test for Self-scaling Variable Metric Algorithms.

M. Al-Baali, University of Damascus, Syria.

In this talk we consider the self scaling BFGS algorithm. We propose a criterion test in which the matrix is prescaled on some iterations before updating and ultimately the regular BFGS steps are used so that the superlinearly convergent property is reserved.

A new approach for the self scaling self dual formula of Oren and Spedicato is also given.

A note on the construction of continuous quadric patches.

M. L. Baart, Potchefstroom University, South Africa.

The simplest approach to the fast graphical display of curved surfaces is to approximate each surface by a number of planar facets. The given surface will, in general, be no more complex than rational bicubic with a rectangular parameter domain. An alternative approach to the use of planar patches is to consider higher order tiles. This means that each small subpatch would no longer be planar, but would be a piece of a higher order algebraic surface. The simplest non-linear algebraic surfaces are the quadrics or second order surfaces. Since the display of each quadric patch will involve considerably more work than the display of a planar patch we will have to improve the image while using fewer of these higher order patches. We will have to ensure at least C_0 continuity between quadric patches. One approach to the approximation of surfaces by continuous curved patches is the use of methods of finite element analysis. A set of linearly independent, non-linear basis functions for a triangle is used to transform this triangle into a curved surface patch in such a way that the boundary curves are uniquely determined by the data on that boundary. This ensures continuity across inter-element boundaries, but the patches are, in general, quartic and not quadric. We consider the conditions required to restrict the order of these patches, and

some properties of the resulting quadrics. A method based on these ideas is proposed for the construction of general quadric patches.

Computing Accurate Eigensystems of Scaled Diagonally Dominant Matrices.

Jesse Barlow and James Demmel, Pennsylvania State University and Courant Institute, USA.

When computing eigenvalues of symmetric matrices and singular values of general matrices in finite precision arithmetic we in general only expect to compute them with an error bound proportional to the product of machine precision and the norm of the matrix. In particular, we do not expect to compute tiny eigenvalues and singular values to high relative accuracy. There are some important classes of matrices where we can do much better, including bidiagonal matrices, scaled diagonally dominant matrices, and scaled diagonally dominant definite pencils. These classes include many graded matrices, and all symmetric positive definite tridiagonal matrices. In particular, the singular values and eigenvalues are determined to nearly full relative precision independent of their magnitudes, and there are algorithms to compute them this accurately. The eigenvectors are also determined more accurately than for general matrices. This work extends results of Kahan and Demmel for bidiagonal and tridiagonal matrices.

Finite Element Approximation of a Free Boundary Problem Arising in the Theory of Liquid Drops and Plasma Physics.

J. W. Barrett and C. M. Elliott, Imperial College and University of Sussex, U.K.

Optimal order error bounds are obtained for a finite element approximation of a variational problem arising in the theory of liquid drops and also in plasma physics. For a bounded domain $\Omega \subset \mathbb{R}^2$ we consider the minimisation of

$$\gamma \langle \nabla \eta, \nabla \eta \rangle + \kappa^2 (1 - \gamma) \langle \eta, \eta \rangle - \kappa^4 \langle G \eta, \eta \rangle$$

subject to $\eta \geq 0$ and $\langle 1, \eta \rangle = M/2$; where $\langle \cdot, \cdot \rangle$ denotes the L^2 inner product, G is the inverse of the Laplacian, $\gamma \geq 0$ and $M > 0$ are given constants. The case $\gamma = 1$ corresponds to a model of a liquid drop sitting on a soap film introduced by Benjamin and Cocker. The case $\gamma = 0$ corresponds to the much studied model plasma problem introduced by Temam.

Conjugate Basis Matrices and Local Convergence for the Algorithm REQP for Constrained Minimisation.

M. C. Bartholomew-Biggs and T. T. Nguyen, Hatfield Polytechnic, U.K.

This paper is concerned with the search directions produced by the sequential quadratic programming method REQP. In particular we consider the components of the search direction in two subspaces which are *conjugate* with respect to the estimated hessian matrix of the Lagrangian function. Viewing REQP in this way leads to a new calculation scheme for the algorithm and also facilitates the analysis of its local convergence properties. Some convergence results will be given together with numerical evidence about the performance of some modified forms of the method.

Multistep Methods for Ordinary Differential Equations based on Algebraic and First Order Trigonometric Polynomials.

G. Vanden Berghe, Rijksuniversiteit Gent, Belgium.

For the numerical integration of an ordinary differential equation (ODE) some multistep methods have been developed which take into account special properties of the solution of the equation. Gautschi(1961) for example constructed methods of the Adams and Störmer type for problems with an oscillatory solution. Also other authors constructed similar methods for ODE's of the type $y' = f(x, y)$ and $y'' = f(x, y)$. These multistep methods integrate exactly trigonometric polynomials (with frequency k) up to a given order and in some cases also algebraic polynomials. The methods are derived in different ways and a discussion of the error terms is not always available. There is a uniform way to construct such multistep methods: the integration of the ODE can be performed by using appropriate interpolation and quadrature rules. We concentrate now on multistep methods with an associated linear difference operator which annihilates not only polynomials up to a certain degree, but also the two functions $\cos(kx)$ and $\sin(kx)$. Therefore we had to construct interpolation rules (and corresponding quadrature rules) which are exact, in addition to polynomials up to a certain degree, for $\sin(kx)$ and $\cos(kx)$. Interesting considerations can be made about the error term and, as a consequence, about the local truncation error of the corresponding multistep method. This error term can be used efficiently in predictor-corrector methods. Numerical experiments show that these multistep methods are accurate. Also good results are obtained, when testing numerically the occurring quadrature rules. These rules, which are easy to implement, are extensions of the quadrature rule of Ehrenmark(1988).

Error Estimation in Automatic Quadrature Routines.

J. Berntsen and T. O. Espelid, University of Bergen, Norway.

A new algorithm for estimating the error in quadrature approximations is presented. Based on the same integrand evaluations that we need for approximating the integral, one may, for many quadrature rules, compute a sequence of null rule approximations. These null rule approximations are then used to produce an estimate of the local error. The algorithm allows us to take advantage of the degree of precision of the basic quadrature rule. In the experiments we show that the algorithm works satisfactorily for a selection of different quadrature rules on all test families of integrals.

A Cahn-Hilliard Type Model for Phase Separation.

J. F. Blowey, University of Sussex, U.K.

Consider a binary alloy, consisting of two species, existing in a state of isothermal equilibrium greater than the critical temperature. Now suppose that the temperature of the alloy is rapidly reduced below the critical value, so that phase separation takes place, where the composition of the alloy changes from being a uniform mixed state to that of a spatially separated structure.

We consider the following model for phase separation: Given $\gamma > 0$ find $\{u(x, t), w(x, t)\}$ such that

$$w = -\gamma \Delta u - u, \text{ when } |u| < 1, \quad \frac{\partial u}{\partial t} = \Delta w,$$

$$u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial \nu} = \frac{\partial w}{\partial \nu} = 0, \text{ for } x \in \Omega.$$

We prove a global existence theorem for a weak formulation of the problem, and then propose a convergent fully discrete finite element approximation which possesses a Lyapunov functional.

For the discrete problem, we show that a subsequence of the solution converges to a critical point of its Lyapunov functional, which confirms that the numerical scheme simulates the asymptotic long time behaviour for the underlying nonlinear evolution equation.

We also display some interesting numerical simulations in one and two dimensions which show that the solution rapidly separates into a two phase structure with interfaces separating the grains, after this rapid evolution, the grains grow and shrink as the interfaces migrate and disappear.

Optimisation of Heavy Oil Recovery.

R. L. Brown, University of Reading, U.K.

Heavy oil can be recovered using the process of cyclic steam injection. Each cycle consists of an injection period followed by a production period. The oil yield from each cycle is dependent upon the length of injection and production periods of the previous cycles.

The development of the steam zone is governed by a weakly singular integral equation which in turn becomes the equation of state in a related control problem.

In this talk we briefly describe the model and a procedure in which the profit from n cycles of the process is maximised for $n \leq z$.

Galerkin Methods for Nonlinear Elliptic PDES.

C. Budd and T. Murdoch, Oxford University Computing Laboratory, U.K.

Many physical systems may be formulated in terms of nonlinear elliptic partial differential equations of the form

$$\Delta u + f(u, \lambda) = 0. \quad (*)$$

Examples include combustion, plasma physics and chemotaxis systems. Such systems may display extremely complex behaviour including multiple solutions, loss of existence for some values of λ and the existence of singular solutions. This behaviour is closely associated with the observation that, if the function $f(u; \lambda)$ grows too rapidly with large u , then in a certain sense the solutions of (*) can not be regarded as stationary points of an appropriate functional. As most Galerkin techniques rely upon this assumption the proofs of the convergence of these methods fail in this case.

We shall demonstrate, however, that Galerkin methods can be successful in computing solutions to (*) and will present a proof of convergence based upon the stability theory of J. C. Lopez-Marcos and J. M. Sanz-Serna.

Stability of Approximations from Radial Basis Function Spaces.

M. D. Buhmann and M. J. D. Powell, University of Cambridge, U.K.

We consider functions of the form

$$s(x) = \sum_{\alpha \in A} c_{\alpha} \phi(\|x - \alpha\|_2), \quad x \in \mathbb{R}^n,$$

where $A \subset \mathbb{R}^n$ is a discrete set and where $\phi: \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$ is prescribed. Such functions are useful as approximations to more general functions in computer calculations when $\phi(r) = r$, for example. The stability question we address is whether large values of the real coefficients $\{c_{\alpha}\}_{\alpha \in A}$ imply large values of $s(x)$ in a local sense. Specifically, we assume that the origin is the only point of A that satisfies $\|\alpha\|_2 < 1$ and that its coefficient is $c_0 = 1$. We ask whether there exists $\Delta > 0$ such that the condition

$$\max_{\|x\| \leq 1} |s(x)| \geq \Delta$$

is obtained where Δ is independent of A and of the coefficients $\{c_\alpha\}_{\alpha \neq 0}$. Our results include numerical values of Δ in two cases where there is an underlying variational problem, namely $\phi(r) \equiv r$ when n is odd and $\phi(r) \equiv r^2 \log r$ when n is even.

An option for implicit Runge-Kutta methods.

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

Although implicit Runge-Kutta methods are usually regarded as most appropriate for stiff problems, they can at least be considered for non-stiff problems. If full implicitness is allowed, it is convenient to aim for a high stage-order and if, for an s -stage method, stage order s is required as well as an overall order of at least s , then such a method is completely specified by the values of $c_1, c_2, \dots, c_s$. In this presentation, some of the possible choices are considered for these quantities. In particular, a choice based on requiring a_{ij} to be constant for $i = 1, 2, \dots, s$ will be discussed. This seems to have some desirable features and some of the properties of the methods defined in this way will be considered.

The Numerical Solution of Large Scale Systems of Differential Equations.

G. D. Byrne, Exxon Research and Engineering Company, USA.

Large scale systems of ordinary differential equations can follow directly from the mechanistic models of complex systems, as in chemical kinetics. More typically, they arise from the application of the numerical method of lines to systems of partial differential equations. This process converts the system of partial differential equations to a system of ordinary differential equations, which can then be solved by one of the modern differential equation software packages. In the case of stiff differential equations, the software must be able to handle the underlying solution of a large scale nonlinear system. In our environment, the stiffness of the system follows from chemical kinetics, diffusion, and long time intervals of integration.

This paper is concerned with some of the techniques that can be used for the numerical solution of large scale systems of stiff ordinary differential equations and indicates areas of current and proposed work. The methods include both direct and iterative types. Tractable examples are included to illustrate techniques that work and techniques that fail. The focus is on the new integrator VODE and the prototypical integrator VODPK, which are written by Peter Brown and Alan Hindmarsh (Lawrence Livermore National Laboratory), and the author. VODE and VODPK are descendants of LSODE and LSODPK and they use direct and Krylov methods, respectively.

Generalised Padé approximations to the exponential function.

F. H. Chipman and J. C. Butcher, Acadia University, Canada and University of Auckland, New Zealand.

We consider an expression of the form

$$G(z; w) = \sum_{i=0}^s P_i(z) w^i$$

with $P_i(z)$ a polynomial of degree n_i , and say that G defines an order N approximation to $\exp(z)$ if

$$G(z; \exp(z)) = O(z^{N+1}).$$

If the coefficients of the $P_s(z)$ are chosen to maximise the order, the approximation is called a generalised Padé approximation. The $s=1$ case gives the usual (rational) Padé approximation. We investigate the A-stability of these approximations for $s > 1$, and present evidence for a generalised version of the Ehle conjecture. We also consider the class of restricted approximations in which $P_s(z)$ has a single zero of multiplicity n_s , and present numerical evidence indicating that only a few of these approximations are A-stable.

Estimation of convergence orders in repeated Richardson extrapolation.
Edmund Christiansen, Odense University, Denmark.

Let $A(h)$ be an approximation depending on a single parameter h to a fixed quantity A , and assume that

$$A - A(h) = c_1 h^{k_1} + c_2 h^{k_2} + \dots$$

Given a sequence of h -values $h_1 > h_2 > \dots > h_n$ and corresponding computed approximations $A(h_i)$ the orders for repeated Richardson extrapolation are estimated, and the repeated extrapolations are performed. Hence the algorithm described can do the same work as Brezinski's E-algorithm, while at the same time providing a check whether repeated extrapolation is justified.

The algorithm is implemented and has proved itself to be a useful tool.

A Tool for Analysing Ill-conditioned Equations.
W. M. Connolly and J. S. Rollett, Oxford University Computing Laboratory, U.K.

Iterative methods for solution of linear simultaneous equations perform badly when the equations are ill-conditioned. If the system of equations is large it can be difficult to understand the reasons for ill-conditioning.

We have used singular value decomposition successfully to analyse such problems and to understand the variations in effectiveness of different methods of preconditioning. The nature of the singular value distribution detects the condition problems, and examination of singular vectors for extreme values gives insight into causes of trouble.

Applications in various fields will be used to illustrate the value of this method of analysis.

The Construction of Cubature Formulae using Software from Bifurcation Theory.
R. Cools, Catholic University, Belgium.

A n -dimensional integral I can be approximated by a quadrature or cubature formula Q

$$I[f] := \int_{\Omega} w(x) f(x) dx \equiv Q[f] := \sum_{i=1}^N w_i f(y^{(i)}).$$

A cubature formula of degree d is by definition a solution of

$$Q[f_j] = I[f_j]$$

where the f_j form a basis for the vector space of all polynomials of degree d or less. The region and the weight function only influences the constants in each equation.

We study cases where the region or weight function contains a parameter. Standard regions can be embedded in a family of regions. We used continuation methods to construct cubature formulae for different values of the parameter, starting from a solution for a specific value of the parameter.

Several unexpected phenomena were observed. For some regions an infinite number of solutions exist. For other regions, bifurcations or turning points occur.

We observe that the structure of the cubature formula changes at turning points and bifurcation points.

Numerical Simulation of the Cahn-Hilliard Equation.

M. I. M. Copetti and C. M. Elliott. University of Sussex, U.K.

In this talk we consider the numerical simulation of the Cahn-Hilliard model for phase separation in a binary alloy. We seek the pair (u, ω) satisfying

$$u_t = \Delta \omega, \quad \omega = -\gamma \Delta u + \psi'(u)$$

in $\Omega \times (0, T)$ with suitable boundary conditions where $\psi(u) = (u^2 - 1)^2/4$. Here u and ω are, respectively, concentration and chemical potential. Numerical experiments with finite difference and finite element approximations in one and two space dimensions show that initial compositions being perturbations of a uniform state in the spinodal interval $(-1/\sqrt{3}, +1/\sqrt{3})$ rapidly evolve into a fine grained structure with interfaces separating phases defined by the uniform values ± 1 . After this rapid evolution into a phase separated structure, a slow coarsening process takes place. In this talk method of approximation and the results of numerical experiments will be described.

Validated Anti-Derivatives.

G. F. Corliss, Marquette University, USA.

We present two approaches to validated one-dimensional indefinite integration: i) find an inclusion of the integrand using Taylor's Theorem with remainder, then integrate this inclusion to obtain an inclusion of the definite integral; and ii) an inclusion of the indefinite integral is computed directly as a linear combination of function evaluations plus an error term using formulas derived from Gaussian quadrature. The approaches presented here have applications in symbolic processors or in special purpose quadrature routines. A numerical example is given.

Multi-Grid Techniques with Non-Standard Coarsening and Group Relaxation Methods.

A. Danaee, International Centre for Theoretical Physics, Trieste, Italy.

In the usual (standard) multigrid methods, doubling of grid sizes with different smoothing iterations (pointwise, or blockwise) have been considered by different authors. Some have indicated that a larger coarsening can also be used, but is not beneficial. In this paper, it is shown that with a suitable blockwise smoothing scheme, some advantages could be achieved even with a factor of $h_{l-1}/h_l = 3$.

The relationship between theorems of the alternative, least square problems, and steepest descent directions.

A. Dax, Hydrological Service, Israel.

This talk reviews the relationship between theorems of the alternative, least squares problems, and the steepest descent directions. It is shown that each of the well known

theorems by Farkas, Gordan, Gale, and others, is related to a certain linear least squares problem that has simple bounds on its variables. Let the vector $\underline{y}$ denote the solution of this problem and let $\underline{r}$ denote the corresponding residual vector. If $\underline{r} = 0$ then $\underline{y}$ solves the "dual" system. Otherwise $\underline{r}$ solved the "primal" system. Moreover, in the latter case $\underline{r}$ solves a certain "steepest descent" problem.

The relationship between theorems of the alternative and least squares problems results in a constructive way for proving these theorems and new theorems of this kind. The relationship with steepest descent problems provides a simple way for calculating the steepest descent vector of constrained polyhedral convex functions. The ability to compute the constrained steepest descent direction provides a straightforward way to resolve degeneracy in active set methods.

Least Squares Data Smoothing by Non-Negative Second Divided Differences.
I. C. Demetriou.

Let n measurements of a convex function be given, where the errors of the measuring process cause convexity to be lost. An algorithm of the following kind is proposed that makes the least square change to the measurements that restores convexity. First, calculate an initial approximation that comes close to the optimum in $O(n)$ operations. Then, use this approximation as the starting point of a suitable quadratic programming algorithm that completes the calculation of the optimum by generating a sequence of infeasible estimates until termination. Each estimate is expressed as a linear combination of linear B-splines, that not only reduces the number of the variables, but also it allows the constraints be satisfied automatically; therefore, the knots of the spline approximations are determined automatically from the data points.

Some Preconditioners for Multi-Vector Processing of Nonsymmetric Systems.
S. Doi, INRIA, France.

Parallel and vector processing algorithms for solving sparse linear systems have been studied for the efficient use of multi-vector computers, such as the Cray-2, Cray X-MP and NEC SX-3 super-computers. Linear systems to be solved are ones arising from finite differencing of 3D advection-diffusion equations.

The preconditioned iterative methods are the most promising class of solution methods. Attention has been focused on parallel and vector algorithms for preconditioners such as the ILU, Incomplete-LU, factorization preconditioners. This is because the rest of the computation is easily parallelized and/or vectorized.

Lichnewsky (1984) has introduced the Nested Dissection technique for parallelising the Incomplete-Choleski preconditioners. Although the method inherits natural parallelism, slight increase in the number of iterations was reported. Duff and Meurant (1988) have recently showed that the VDV-ordering, which is named after Van der Vorst and for use on 2D rectangular grids, has stability and sometimes better convergence characteristics than the normal typewriter ordering. The authors (1987) have introduced the Tridiagonal Factorization (TF) algorithm as an ADI-like preconditioner for parallel and/or vector processing.

In this paper, two 3D ordering methods are first introduced as extensions of the 2D VDV-ordering. One has 4-parallelism and the other has 8-parallelism. These methods are implemented using the Nested Dissection technique, in order for achieving larger granularity of parallelism. In each 'nested' sub-domain, two different vectorization techniques are introduced: the diagonalwise vectorization technique and the hyperplane vectorization technique. The Tridiagonal Factorization method and some other new

methods are also implemented. The Conjugate Gradient Squared method (Sonneveld (1984)) is used as the basic iterative procedure for nonsymmetric systems.

Comparison of convergence has been made using some advection-diffusion equations. It is shown that the parallel ILU preconditioner with 8-parallelism has better convergence features not only than the other parallel preconditioners but also than the typewriter-ordered preconditioner, which is most commonly used on scalar computers. The 8-parallelism method has another substantial feature; i.e., the method has 'numerical symmetry' equivalent to the geometric symmetry of the cubic domain. Comparison of computational speed on the CRAY-2 multi-vector computers will also be presented at the conference.

Parallel Hopscotch Solutions of the Ginzberg-Landau Equation.
D.B. Duncan, Heriot-Watt University, Edinburgh.

The Hopscotch method was very popular in the early 70s for the approximation of parabolic PDEs (see Mitchell and Griffiths, "The Finite Difference Method in PDEs" for references to papers by Gourlay, McGuire, Mitchell, Morris etc.). Although the Hopscotch method is not the most efficient method for use on standard sequential computers, this evaluation is not so clear cut for parallel computers. However, it is clear that programming a parallel version of the Odd-Even Hopscotch is much easier than programming its competition (e.g ADI). Further, it has "nearest neighbour" data dependence which is ideal for implementation on a variety of parallel computer architectures. We shall concentrate on its implementation on an array of INMOS Transputers.

We use the Ginzberg-Landau equation:

$$u_t = \epsilon^2 \Delta u + u(1-u^2)$$

as an illustrative example (in two space dimensions). This nonlinear PDE has solutions which evolve extremely slowly and require time steps over a huge range of values. The Odd-Even Hopscotch method has a natural time step control which copes with this and it produces affordable results.

We hope to demonstrate that the Hopscotch method is efficient enough and (perhaps more importantly) easy enough to program for use as an investigative tool in the solution of suitable PDEs on parallel computers.

Optimal Distribution of Knots in Tensor-Product Splines Approximation.
N. Dyn and I. Yad-Shalom, Tel-Aviv University, Israel.

Known results on the optimal distribution of knots, which asymptotically minimises the $L_p[0,1]$ error in spline approximation of a sufficiently smooth function, are extended to the following cases:

- (1) An optimal distribution for a simultaneous $L_p[0,1]$ approximation of a finite set of functions, or a set which depends on a continuous parameter.
- (2) An optimal distribution on each axis for $L_2[0,1]^2$ tensor-product spline approximation. This result extends to $L_2[0,1]^n$, $n > 2$.

An algorithm for tensor-product knots placement based on the theoretical optimal distributions is designed and tested. It seems that this algorithm produces nearly optimal knots in case of a large or moderate number of knots (as in the case of the univariate setting), and is superior to existing heuristic methods.

On Positive Shock Capturing Schemes.

B. Einfeldt, Cranfield Institute of Technology, U.K.

A major problem in the design of modern shock capturing schemes is the specification of stability-criteria which guarantee oscillation free numerical results. While there are several potentialities to construct second order accurate TVD schemes in one space dimension, no such schemes exists in two space dimension - at least if we use a straightforward extension of the TVD-condition to two space dimension. Therefore, the popular second-order accurate Finite Volume schemes do not belong to the class of TVD-schemes.

In the present paper we give a short survey of the design-principles for Positive schemes and discuss the relation to TVD and Classical shock capturing schemes.

Discretisation and Asymptotic Behaviour of Dissipative Dynamical Systems.

C. M. Elliott, University of Sussex, U.K.

We shall consider dissipative dynamical systems generated by nonlinear evolution equations of the form

$$Bu_t + Au + f(u) = 0, \quad u(0) = u_0$$

(where B and A are symmetric positive semidefinite linear operators), which possess an absorbing set and/or a Lyapunov functional. Such abstract equations are obtained from 'parabolic' equations such as

- a) Reaction diffusion $u_t = \Delta u + u - u^3$
- b) Cahn-Hilliard $u_t = \Delta w, \quad w = -\gamma \Delta u + u^3 - u$
- c) Phase Field $\theta_t + \lambda u_t = \Delta \theta, \quad \tau u_t = \gamma \Delta u + u - u^3 + \theta$

We are interested in showing that certain time discretizations yield approximations which possess long time behaviour similar to that of the evolution equation.

Comparison of Roe's Scheme and a Directional Difference Scheme for Gas Network Flows.

S. Emmerson, University of Reading, U.K.

Two numerical schemes for systems of hyperbolic conservation laws, namely, Roe's scheme which uses an approximate linearised Riemann solver, and the directional difference scheme, which is a pseudo-characteristic variable method used in the gas industry, are compared and contrasted. Each scheme is applied to a test problem typifying conditions in gas transmission networks.

Software for Adaptive Multidimensional Integration.

T. O. Espelid, University of Bergen, Norway.

A new algorithm for multidimensional (n-cube) numerical integration has been developed by Bernsten, Espelid and Genz (1988). The main aim has been to develop an algorithm that is more reliable than the available software in this field. This is achieved mainly through a more sophisticated error estimating technique. In addition we decided to offer more than one integration rule in each dimension, based on the experience that the relative performance of different rules may change from one problem to another. The main difference between optional rules is the polynomial degree. The algorithm uses a global adaptive subdivision strategy and has been structured to allow efficient implementation on shared memory parallel computers. A FORTRAN

implementation of the algorithm (ADMINT) has been tested on an Alliant FX/8 and some test results will be presented. In addition the code has been successfully run on SUN 3/50, CRAY-XMP/48, IBM 3090, Sequent Balance 8000 and HP-9000/840.

Multistep Methods based on Continued Fractions for solving Initial Value Problems.
D. Eyre and S. Abelman, Potchefstroom University and University of the Witwatersrand, South Africa.

Rational multistep methods of both osculatory and Adams type are investigated for solving initial value problems of ordinary differential equations. The formulas are given in a form suitable for variable step calculations. Some local truncation errors are provided. Numerical tests of the performance of the methods including a computational investigation of the regions of absolute stability and the numerical treatment of two equations with singular solutions is presented.

A deficient spline function approximation to third order O.D.E.
T. Fawzy, Suez-Canal University, Egypt.

A method for approximating the solution of the initial value problem: $y''' = f(x, y)$ using spline polynomial of degree m is presented. The method is shown to be convergent for $m = 7$ and 8. In addition, global error bounds of the form:

$$\|s^{(i)}(x) - y^{(i)}(x)\|_{\infty} = O(h^{m+1-i}), \quad i = 0(1)m$$

are presented as well as the consistency of the procedures, where the function $f \in C([a, b] \times \mathbb{R})$.

Thin Plate Spline Approximants,
P. Gonzalez-Casanova, University of Oxford, U.K.

This work is divided in two parts. In the first part we study the problem of approximating in a local way the value of an arbitrary function prescribed in the nodes of a finite regular grid. Here by local we mean that the value of the unknown function at an arbitrary point can be approximated by considering only some of the originally prescribed data. The method we present here uses thin plate splines and can be interpreted as a generalisation of the variation diminishing spline of Schoenberg. We based our construction on two different approaches: spline approximants in Hilbertian subspaces of $H^2(\Omega)$, by Benbourhim (1986); and a formulation developed by Nira Dyn et al (1983-86). In Nira Dyn's work a generalisation of the unidimensional B-spline is formulated by constructing a bell shape function that is a linear combination of the fundamental solution of the biharmonic operator. On the other hand in the work of Benbourhim a new concept of spline approximants is developed by constructing a surface that converges pointwise to the unknown function. Our aim is to combine Benbourhim's spline approximants approach with Nira Dyn's B thin plate splines in such a way that the resulting surface can be used to approximate the function in a local way. In this first part we also show the relation that exists between spline approximants and the variation diminishing spline of Schoenberg.

In the second part we treat the problem of approximating an unknown function that is prescribed at the vertices of an arbitrary regular and affine triangulation. In this part we overcome one of the practical limitations of Benbourhim's work: that the approximating surface depends on the generally unknown reproducing kernel of $H^2(\Omega)$. We construct a surface that converges pointwise to the data function and depends only on the fundamental solution of the biharmonic operator.

Stable solvers for singular linear systems and application to block linear systems.
W. Govaerts, University of Gent, Belgium.

G. Moore and A. Spence (The calculation of turning points of nonlinear equations; SIAM J. Numer. Anal. 17 (1980) 567-576) consider a block linear system of the form

$$\begin{bmatrix} A_{11} & A_{12} & A_{13} \\ 0 & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \end{bmatrix}, \quad x_1, x_2 \in \mathbb{R}^n, x_3 \in \mathbb{R},$$

or $Mz = h$, where M is well-conditioned. J.D. Pryce (personal communication) suggested to solve this system by principally using given solvers for systems with A_{11}, A_{22} and their transposes in spite of the obvious difficulty that A_{11} and A_{22} are nearly singular.

We present an algorithm that uses 2 solves with each of A_{11} and A_{11}, A_{22} and 1 solve with each transpose, totalling 6 solves with possibly singular or nearly singular systems. The solvers may be based on direct or iterative methods; it is required only that they be backward stable in the sense of J. Wilkinson.

The present algorithm contains as a special case a solution for a bordered singular linear system. Such systems have received much attention in the literature (T.F. Chan and others) because of their interest in numerical continuation.

Solution of Elliptic Systems of P.D.E.'s by Cell Discretization.
J. Greenstadt, University of Cambridge, U.K.

The Cell Discretization algorithm is applied in a straightforward manner to a few very simple elliptic systems of partial differential equations. The discrete approximant of the solution depends, as usual, on sets of coefficients of intracell basis functions, one set for each cell. The usual transformation to new variables, one subset associated with interfaces and the other with cells, is easily generalised to the multivariable case. This renders the calculation almost entirely cellwise independent, and therefore readily parallelizable without special reorganisation. The residual dependency in the calculation is the solution of the system of equations for the interface variables, which is done in the computer program by a preconditioned conjugate gradient method on the normal equations. Results for a simple gradient-divergence system, the Cauchy- Riemann equations, a Stokes problem and the clamped plate problem are shown in graphic form.

On Approximate Solutions of Integral Equations of the Mixed Type
L. Hacia, Poznan University, Poland.

Consider the following integral equation

$$f(x, t) + \iint_{OM} N(x, t; y, s) f(y, s) d\mu(s) = g(x, t), \quad t \in [0, T],$$

where g is a given function in $W = M \times [0, T]$, N is a kernel defined in $W \times W$ and f is an unknown function. Here M means a sufficiently regular and compact manifold in $\mathbb{R}^m$ ($m \geq 2$) and μ is the measure function on manifold M .

For approximate solution of that equation we apply method of the partition of the unity, methods of the Galerkin type and method of the Fourier type. It is proved the convergence and the error estimate is established.

Some initial - boundary problems for a number of differential partial equations of physics, mechanics and technology are reducible to the equation (for example, Fourier

problems for linear equations of parabolic type).

Highly Continuous Runge-Kutta Interpolants.

D. J. Higham, University of Toronto, Canada.

To augment the discrete Runge-Kutta solution to the initial value problem, piecewise Hermite interpolants have been used to provide a continuous approximation with a continuous first derivative. We show that it is possible to construct interpolants with arbitrarily many continuous derivatives which have the same asymptotic accuracy and basic cost as the Hermite interpolants. We also show that the usual truncation coefficient analysis can be applied to these new interpolants, allowing their accuracy to be examined in more detail. As an illustration, we present some globally C^2 interpolants for use with a popular 4th and 5th order Runge-Kutta pair of Dormand and Prince, and we compare them theoretically and numerically with existing interpolants.

Trajectory Optimisation Applications using the Program STOMP for Generating Cost Function and Gradient Evaluations.

K. Horn, Messerschmitt-Boelkow-Blohm, Germany.

A fortran program is discussed for use in trajectory optimisation for the constrained optimal control problem. The package delivers cost function and gradient estimates for use by a parameterised optimisation method. Emphasis is given to means of improving accuracy in the gradient estimates as well as to reducing computing time. Runge-Kutta methods are used to solve the ordinary differential equation systems, treating these systems in a straightforward fashion. Such an approach permits a simple formulation for problems in which time related discontinuity points are to be located optimally, e.g., the time at which to activate sharp rolls, thrust run-up/run-down, braking devices, etc. The use of an embedded root solver gives the same ease in handling dependent variable related discontinuities. Inherent in this formulation is the ability to "break away" from the prescribed control functions when algebraic constraints are violated. Features are incorporated for improving the flexibility of the control function structure, including the use of movable grid points for modelling near discontinuities in the control functions, for activating switching times in the controls, etc. Means of achieving high accuracy in the gradient estimates are discussed, and conditions under which different approaches break down are given. Applications are presented from aircraft trajectory analysis.

Embedded Runge-Kutta Methods on Parallel Computers.

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

By explicit Jacobi-type or diagonally implicit iteration of high-order Runge-Kutta methods it is possible to construct high-order explicit and diagonally implicit Runge-Kutta methods containing embedded formulas of lower order and possessing a high degree of parallelism. We construct:

- (i) explicit, p th-order methods requiring p sequential stages, for any value of p .
- (ii) diagonally implicit, L -stable, p th-order methods requiring p sequential stages, for $p \leq 6$ and $p = 8$.
- (iii) diagonally implicit, $A(\alpha)$ -stable, p th-order methods with $\alpha = \pi/2$ and requiring $p-1$ sequential stages, for $p = 3, 5, 7$.

All methods require $\lceil (p+1)/2 \rceil$ processors and contain embedded formulas of orders $p-1, p-2, \dots$. This work was done jointly with B. P. Sommeijer and W. Couzy.

Some New Ideas on Conjugate Gradient Methods.

Y. F. Hu and C. Storey, Loughborough University of Technology, U.K.

Recently Liu and Storey suggested a new conjugate gradient algorithm for unconstrained optimisation which seems more efficient than the usual conjugate gradient algorithms, limited numerical results also show that the new algorithm is compatible with Quasi-Newton methods. We look at an embedded conjugacy idea in the algorithm and the prospect of using this to form new algorithms. An N -step quadratic convergence property of Liu's algorithm is also considered.

Unconditional Convergence of some Crank-Nicholson LOD Schemes.

W. Hundsdorfer, CWI, Amsterdam.

Discretization in space of parabolic initial-boundary value problems in several space variables leads to large systems of ODEs.

$$\dot{u}(t) = F(t, u(t)),$$

where F will depend on the grid distances Δx in space; for small Δx the system will become very stiff. The function F can often be split in a natural way as $F = F_1 + F_2 + \dots + F_s$, with each F_j corresponding to space derivatives in one direction.

The use of an implicit numerical method, such as the Crank-Nicholson scheme, to solve the differential equation, requires solution of very large algebraic systems. With the so-called splitting methods, such as Locally One Dimensional (LOD) schemes, the multi-dimensional computations are replaced by a series of more simple one-dimensional computations.

For the convergence analysis of splitting methods it is often assumed that Δx is fixed. We shall consider unconditional convergence where both Δx and the time-step Δt may tend to zero, independently of each other. It is known that this may affect the order of discretization errors; due to stiffness an order reduction can occur. In this talk it will be analysed to what extent the local and global discretization errors will be affected.

The Numerical Solution of Parabolic Free Boundary Problems Arising From Thin Film Flows.

R. Hunt, University of Strathclyde, U.K.

A numerical solution of high accuracy is obtained for the large Reynolds number, thin film flow over a horizontal flat plate, cylinders and spheres resulting from a vertical jet of fluid falling on the surface. A co-ordinate transformation is used which simultaneously maps the film thickness onto the unit interval and removes the singularity at the leading edge. The resulting equations are parabolic and these are solved using the Keller box method which is modified to accommodate the outer, free boundary. Using an extrapolation technique, results of sixth order accuracy are obtained with an estimated accuracy of six significant figures. For the flat plate, solutions for both two-dimensional and axisymmetric jets are obtained and, for cylinders and spheres, different Froude numbers and volume flows are considered. Finally, the three dimensional flow resulting from a cylindrical jet impinging onto the top generator of a cylinder will be presented.

Equilibria of Runge-Kutta Methods.

A. Iserles and J. M. Sanz-Serna, University of Cambridge and University of

Valladolid, Spain.

It is known that certain Runge-Kutta methods share the property that, in constant-step implementation, their fixed points are exactly the fixed points of the underlying ODE. In other words, if a solution trajectory tends to a bounded limit then it is always asymptotically "correct". Such methods are called *regular*. In this talk we present a recursive regularity test, as well as a necessary condition on the characteristic polynomial of the Runge-Kutta matrix. These are implemented to characterise all regular 3-stage methods of order ≥ 3 , all regular Gauss, Radau and Lobatto schemes and all regular quasi-implicit methods (e.g. SDIRK, DIRK and SIRK). We also debate implications of the theory to variable-step implementations.

Constrained Moving Finite Elements using Piecewise Cubics in 2-d.
P. Jimack, University of Bristol.

In this paper we describe the implementation of a finite element formulation using reduced Hermite cubic basis functions on a continuously adapting triangulation, for the solution of a genuinely 2-d moving boundary problem arising in silicon crystal growth.

The basis functions, $\alpha_j(\underline{x}, \underline{x}(t))$ say, are time dependent, so differentiating the approximate solution with respect to time yields terms of the form $(d\alpha_j/d\underline{x})(d\underline{x}/dt)$. An expression is derived for these derivatives of α_j with respect to grid movement for this basis, and it will be indicated how such an expression may be simply achieved for any finite element basis. This expression is then incorporated neatly into the finite element algorithm to allow the efficient solution of the problem.

In this particular application the grid deformation is governed by the motion of the boundary, which, in turn, depends on the local gradient of the solution. The reduced Hermite space is chosen to give accurate representation of this gradient.

L_∞ Errors in Finite Volume Approximations.
R. Jones, University of Oxford, U.K.

In this paper an L_∞ error expression is derived for bilinear approximations to a model Poisson problem. From this the error in the finite volume approximation is shown to be as good as the finite element error, though with slightly more restrictive regularity conditions. Numerical results to demonstrate the theoretical predictions are then given.

On Optimally High Order in Time Approximations for the Korteweg-de Vries Equation.
O. Karakashian and W. McKinney, University of Tennessee, U.S.A.

We consider the problem of approximating periodic solutions of the Korteweg-de Vries (KdV) equation. These approximations use a Finite Element - Galerkin process for the spatial discretization and Implicit Runge-Kutta (IRK) methods for the temporal discretization, our main concern here being the temporal rate of convergence.

It is well-known that for some problems, the observed rate of convergence is lower than the classical rate, which we may define as the rate expected when applying the same method to a linear problem. This is the so-called order reduction phenomenon. In the case of the KdV equation, in a previous paper, the order reduction was nullified by the introduction of appropriate correction terms during the calculation of the intermediate values for two diagonally implicit methods of (classical) rates of 3 and 4. We

have recently shown that these modifications were unnecessary, i.e. the classical rates are achieved. In particular, we obtained the rate of $2q$ for the q -stage Gauss-Legendre methods. This is in perfect agreement with the results of numerical experiments.

The novel approach used in proving the convergence rates can be extended to other interesting equations, such as the Nonlinear Schrödinger equation.

An Interval Step Control for Continuation Methods.

R. B. Kearfott, University of Southwestern Louisiana, U.S.A.

Continuation methods can be important tools for analysing parameter-dependent physical systems, for performing geometric deformations, and for solving nonlinear systems of equations. Some applications may require reliable methods in the sense that it is mathematically impossible for them to cross from one component of the solution to another. We will discuss such a technique in this talk.

We first briefly review continuation methods in general. We then outline the underlying principles of interval arithmetic which enable us to construct a reliable algorithm. We describe the algorithm and state our theoretical results, then present some preliminary experimental comparisons. Finally, we draw conclusions and speculate on future development.

Sub-lattices of Integration Lattices.

P. Keast, J. N. Lyness and T. Sorevik, Dalhousie University, Canada, Argonne National Laboratory, USA and University of Bergen, Norway.

Integration lattices are special sets of points which may be used to approximate to integrals over the unit hypercube in s dimensions. For some applications it is useful to have a sequence of lattices $L(i)$, with $L(i)$ embedded in $L(i+1)$, thus providing a sequence of approximations to the integral which may be used to obtain error estimates. Given the generating matrix of a lattice, however, identification of sub- or super-lattices is not generally a simple matter. The generation of sub- and super-lattices is made easier by examining the reciprocal lattice, whose points are all integers. A characterisation of all lattices of a given order, and of all sub- and super-lattices will be given. An algorithm will be displayed for the generation of all sub-lattices of a given lattice.

Parallel Evaluation of Some Recurrence Relations by Recursive Doubling

Ayşe Kiper and D. J. Evans. Middle East Technical University, Turkey and Loughborough University of Technology, UK.

A class of second order linear recurrence formulae result from the Fourier series coefficient of the Jacobian elliptic functions $sn^m(u, k)$, $cn^m(u, k)$ and $dn^m(u, k)$ with $m \geq 1$. The parallel evaluation of these coefficients are obtained by recursive doubling procedure and various aspects of the computations and results are compared and discussed with those obtained by nested recurrent product form algorithm and sequential algorithm.

Solution of exterior Helmholtz problems by improved boundary element methods.

S. M. Kirkup, Brighton Polytechnic, U.K.

In this presentation we consider the problem of solving the Helmholtz equation:

$$\nabla^2 \phi(p) + k^2 \phi(p) = 0, \quad p \in E$$

in a region E exterior to a bounded boundary S with a boundary condition defined on S which is most generally of the form

$$a(p)\phi(p) + b(p)\frac{\partial\phi}{\partial n_p}(p) = c(p), \quad p \in S$$

and the satisfaction of a condition (a radiation condition) on ϕ at infinity. The techniques we consider for solving this problem are, what we term, the improved boundary element methods. Early researchers attempted a numerical solution of the exterior problem using methods based on straightforward integral equation formulations (such as those termed the Helmholtz integral equation or the Helmholtz-Kirchoff integral equation in the literature or those derived via simple layer potentials). However, these formulations were found to be unsuitable as the basis for numerical methods because of either non-existence or non-uniqueness of their solution at certain values of k related to the geometry of the boundary. Methods were then developed for alleviating these problems, the most important of which is the one introduced in Schenck (1968).

The improved boundary element methods are those based on either the indirect integral equation formulations introduced by Leis (1965), Panich (1965), Kussmaul (1969) or the direct formulation introduced by Burton and Miller (1971). Each of these formulations contain a free parameter (a complex number). For Dirichlet problems ($b(p)=0$) and Neumann problems ($a(p)=0$) these formulations of the Helmholtz problems have a unique solution at all values of k provided the free parameter has an imaginary component. For the more general Robin boundary condition the existence and uniqueness of a solution has not been proven.

Although the condition on the free parameter for the integral equation to have a unique solution is a weak one it is found that much firmer control of the parameter must be taken in the implementation of the boundary element method if it is to work satisfactorily. It is this problem that will mainly be discussed in the presentation. Kress and Spassov (1983) suggested ideas for choosing the free parameter and these will be criticised. Testing on different choices of parameter was carried out when the boundary is a sphere and the boundary condition is axisymmetric. The results from these tests will be presented. Further guidance in the choice of weighting parameter is given.

A reliable boundary element method for the solution of the generalised Robin problem is considered.

A Regularization-Technique for the Numerical Solution of Index-2 - Differential-Algebraic Equations

Michael Knorrenschild, Lawrence Livermore National Laboratory, USA.

We consider initial value problems in index-2 differential-algebraic equations (DAEs)

$$y'(t) = f(y(t), z(t)), \quad 0 = g(y(t))$$

where $y(0), z(0)$ are given, and $y(t) \in \mathbb{R}^m, z(t) \in \mathbb{R}^{n-m}$ are unknown and $(g'(y)f_z(y, z))^{-1}$ exists. The proposed technique is to introduce a small parameter $\epsilon > 0$ into the system in a way that the resulting system has index-1 and therefore is easier to solve numerically.

We investigate the numerical behaviour of Runge-Kutta methods applied to a model problem and give conditions under which the numerical approximation for the perturbed system permits error bounds that are uniform in ϵ near 0. Numerical experiments suggest that it has advantages to solve the perturbed system numerically rather than the unperturbed form.

Chebyshev Polynomial Solutions of First Kind Integral Equations for Numerical Conformal Mapping.

J. Levesley, D. M. Hough and S. N. Chandler-Wilde, Coventry Polytechnic, U.K.

A numerical method is described for the conformal mapping of simply connected domains whose boundaries contain sharp corner points onto the exterior or interior of a unit circle. The method is based on a first kind integral equation formulation due to Wendland (in numerical Treatment of Integral Equations, Birkhauser Verlag, 1980 (J. Albrecht and L. Collatz, editors)). On each component analytic arc of the boundary the unknown source density divided by the Chebyshev weight function is approximated by a finite Chebyshev polynomial series. The coefficients in these series are determined by collocation. The advantage of the method is efficiency in the setting up of the linear algebraic system which approximates the integral equation; the boundary integrals which arise are evaluated by a combination of analytic integration and an FFT, making use of properties of the Chebyshev polynomials. A partial convergence analysis of the method is given. The calculation of the inverse map is also discussed and the application of the mappings to the problem of orthogonal boundary-fitted mesh generation is briefly described. Numerical examples to illustrate the accuracy of the numerical methods are given.

New Stopping Criteria for Some Iterative Methods for a Class of Unsymmetric Linear Systems.

C. Li and D. J. Evans, Loughborough University of Technology, U.K.

When the iterative procedure $x_{k+1} = Gx_k + g$ for the linear system $Ax = b$ is considered, one of the important items for the method is the stopping criterion. Usually, we use one kind of norm as a measure and if the norm of the pseudo-residual vector $\delta_k = Gx_k + g - x_k$ is small, then we terminate the iterative procedure. However, this does not guarantee that the norm of the error vector $e_k = x_k - x^*$ ($x^* = A^{-1}b$) is small. In this paper, we wish to show that if there exists a nonsingular matrix Z such that ZGZ^{-1} is skew-symmetric, then we have $\|e_k\|_Z \leq \|\delta_k\|_Z$, $\|y\|_Z = \|Zy\|_2$. The relative error bound is also given. The applications of the results to the GCG method and Chebyshev acceleration are included.

On a Certain Approximation problem for Matrices.

W. Light, University of Lancaster, U.K.

We will consider the problem of approximating a matrix C by matrices of the form $AX + YB$. Here A and B are fixed matrices, and we seek X and Y such that

$$\|C - (AX + YB)\|$$

is minimised for some norm. Areas where this problem arises will be described as well as algorithms for the solution in certain cases. The algorithms seek to take advantage of the inherent structure in the problem.

The Whittaker-Henderson graduation method

A. J. Macleod, Paisley College, Glasgow.

The graduation, or smoothing, of mortality rates to produce life tables is an important problem in actuarial mathematics. Given a set of observed rates p_i , $i = 1, \dots, n$ the Whittaker-Henderson method produces graduated values g_i , $i = 1, \dots, n$, by

minimising the function.

$$\sum_{i=1}^n w_i (p_i - g_i)^2 + \alpha \sum_{i=1}^{n-p} [\Delta^p g_i]^2.$$

The optimal value of α can be chosen by cross-validation. We discuss the theoretical and computational aspects of this problem and illustrate them with data used in the English Life Tables no 13.

Differential and integro-differential equations as population growth models with applications in Agriculture.

A. Makroglou, Agricultural University of Athens, Greece.

Differential and integro-differential equations have applications in various scientific areas such as Physics, Chemistry, Control theory, Biology, Demography, Epidemiology.

Here are given examples of Demography applications concerning the dynamics of populations governed by birth and death processes with interest to Agriculture. Such populations include livestock, wildlife, fish, insects, bacteria. Depending on whether the age of the populations is taken into account we have ordinary or partial differential and integro-differential equations. Most of the work published is concerned with deterministic models. Less work appears to have been done with stochastic models.

Fast, Reliable Numerical Algorithms for Sturm-Liouville Computations.

M. Marletta and J. D. Pryce, RMCS Shrivenham, U.K.

There is presently a dearth of library software for frequently occurring computations associated with Sturm-Liouville problems.

$$-(p(x)y')' + q(x)y = \lambda w(x)y \quad (a < x < b).$$

Such computations include (i) finding eigenvalues and eigenfunctions. (ii) counting the number of eigenvalues in a range $[\lambda_{\min}, \lambda_{\max}]$ (iii) computing so called quasibound states and resonance energies (these problems arise in quantum theory) and (iii) computing moments involving eigenfunctions (Fourier Integrals, Franck-Condon factors).

Much of the software for these problems has been written by quantum physicists, and is typically highly problem specific; little (if any) has undergone the rigorous testing carried out on library software, or has found its way into widely available program libraries. We are designing a package of routines which should be general in their applicability and have already proved less expensive to use than existing library software.

For the basic discretization we have adopted the Pruess method, which replaces the coefficients in the Sturm-Liouville differential equation by piecewise polynomials. We use piecewise constants (PWC's) despite the low $O(h^2)$ convergence, this has yielded surprisingly good accuracy at low cost. We have developed an apparently good automatic meshing algorithm, and a remarkably simple, effective algorithm for truncating the interval near a singular point, which seems to be better than some more sophisticated (problem-specific) techniques.

The Effect of Filtering on the Pseudospectral Solution of Evolutionary Partial Differential Equations.

L. S. Mulholland, University of Strathclyde, U.K.

This paper examines the effect of filtering on the solution of time-dependent partial differential equations by the pseudospectral method. It is shown that if spatial discretisation is effected using the Fourier pseudospectral method the computed solution will be an approximation to the solution of a modified differential equation. The changes in dispersive and dissipative properties induced by the modification are examined, and numerical results are presented which illustrate these changes for both linear and nonlinear equations. Numerical results are also presented which show the effect of filtering on Chebyshev pseudospectral solutions of time-dependent equations.

Galerkin and Petrov-Galerkin Methods for the Semiconductor Problems.
T. Murdoch, University of Oxford, U.K.

We address the problem of solving the one dimensional steady state semiconductor equations within a Galerkin framework. These comprise three highly nonlinear, coupled differential equations for the electrostatic potential ψ and the Fermi-potentials ϕ_p and ϕ_n . In preference to discretizing the differential equations by the finite element method and solving the resulting nonlinear algebraic equations by Newton's method, a Newton linearisation of the differential equations is performed and a sequence of linear, elliptic equations solved until convergence is reached.

The linear equations associated with ϕ_p and ϕ_n are non-self-adjoint and consequently the Galerkin method in its crude form does not adequately approximate them. However, by using the Petrov-Galerkin techniques of Barrett and Morton (1984), we show that a near optimal test space can be chosen at each step of the Newton iteration: moreover, the resulting Petrov-Galerkin approximation is near optimal in a norm closely related to the standard L_2 norm. Numerical results are presented to demonstrate the effectiveness of this approach.

Preconditioned Conjugate Gradient Methods for Equality Constrained Least Squares Problems.
N. K. Nichols, University of Reading, U.K.

Faber polynomials on circular sectors.
G. Opfer, University of Hamburg, F. R. Germany.

According to work by S. Ellacott (Math. Comp. 40(1983), 575-587) and by J. P. Coleman and R. A. Smith (Math. Comp. 49(1987), 231-241, S1-S4) it is possible to construct the Faber polynomials on circular sectors recursively. This recursion, however, is rather involved. Therefore, the latter two authors have given numerical values for the coefficients for certain opening angles of the sectors. It will be shown that by applying some sort of brutal force (i.e. certain computer programs) it is possible to derive the coefficients explicitly in terms of the (arbitrary) opening angle. This work has been done in cooperation with Christoff Hoffmann (Purdue) and Karin Gatermann (Hamburg).

New families of convergence acceleration methods: The P-algorithms.
K. J. Overholt, University of Bergen, Norway.

We describe new infinite families of convergence acceleration algorithms, designed for a class of sequence typified by (generalised) power series or more generally any sequence satisfying a certain regularity requirement. The notion of P-order is introduced as a measure of the efficiency of convergence acceleration methods. A distinguishing feature of the new algorithms is that they use not only the numerical values

of the sequence members but also structural parameters contained in the regularity requirement. Theorems about the existence or non-existence of P-algorithms of prescribed P-order are proved. The new algorithms are simple and compare favourably with known methods.

A Quadratically Convergent Parallel Jacobi-like Eigenvalue Algorithm.
M. H. C. Paardekooper, Tilburg University, The Netherlands.

This paper describes a new Jacobi-like diagonalisation process for non-normal diagonally dominant matrices. It is quadratically convergent. In each step $n/2$ (assume n to be even) pairs of symmetrically placed off-diagonal elements in a $n \times n$ matrix are annihilated by a transformation with a direct sum of 2×2 matrices. Each 2-dimensional unimodular shear annihilates a 2×2 submatrix. These shears are not unitary. Consequently, the monotonic decrease of the off-diagonal part cannot be guaranteed. We prove that this Jacobi-like annihilation process converges quadratically to a diagonal if the nondiagonal part is sufficiently small relative to the separation of the eigenvalues. In case of multiple eigenvalues the proof is based on theorems of Fan & Hoffman (1954) and Wilkinson (1968).

Our method can be parallelised (hypercube, systolic array), as the Jacobi process for the symmetric eigenproblem. For matrices with a large departure of normality, the annihilation procedure can be used as final stage in the improved version of Sameh's (slowly convergent) parallel normreducing eigenvalue algorithm.

Numerical examples will be given to illustrate the theoretical results.

Using Divergent Iterations in High Speed, High Accuracy Computations.
P. Pedersen, Technical University of Denmark.

To find a solution x^* to an equation $F(x)=0$, you replace the equation by an equivalent iterative form $x=g(x)$, and in the textbooks the iteration $x_0 := APPROX(x^*)$, $x_{n+1} := g(x_n)$ converges to x^* - otherwise you use it for making (nice) coloured pictures.

However, for the average computer it is often difficult to find a suitable g : the iteration may be too slow, even divergent, or computing $g(x_n)$ with the accuracy needed may be too complicated - especially in the N dimensional or infinite-dimensional case.

In the talk I shall discuss how to use g -functions which are simple to find and simple to compute - even if the corresponding iteration is divergent in the traditional sense.

FFT solution of the Robbins problem
W. M. Pickering and P. J. Harley, University of Sheffield.

FFT methods are well established as efficient methods for solving a certain class of partial differential equations with Dirichlet, Neumann or periodic boundary conditions. In this note it is demonstrated that, by a perturbation of the appropriate eigenfunction expansion, an algorithm can be devised for the case of Robbins boundary conditions, for which the usual FFT methods are unsuitable.

Numerical results are presented for a model problem and the extra computational cost, compared with established cases, is shown to be relatively small.

Reliable Computation of Weyl's $m(\lambda)$ Function.
J. D. Pryce, M. Brown and V. Kirby, RMCS and U.C. Cardiff.

The $m(\lambda)$ function of a Sturm-Liouville problem (SLP) was central to Weyl's analysis of the spectral theory of SLP's. It is an analytic function that has more recently found other applications, notably to a classic pure mathematical problem: Find the best constant K in Hardy-Everitt-Littlewood Polya (HELP) inequalities

$$\left[\int_a^b (p |f'|^2 + q |f|^2) \leq K \int_a^b w |f|^2 \right] \left[\int_a^b \frac{1}{w} |-(pf')' + qf|^2 \right]$$

(where $p > 0$, q real, $w > 0$ are given functions and f is an arbitrary function).

The original 1932 result of H, L & P was that when $p=1$, $q=0$, $w=1$ then (best) $K=4$. More general cases resist analytical methods and involve computing $m(\lambda)$ numerically. We describe our efforts to develop an algorithm that does this over a wide area of the λ plane, and an algorithm with error control that has proved remarkably successful over a "reasonable" area of the plane.

The Solution of Semi-infinite Programming Problems by Discretization Methods.

R. Reemtsen, Technical University of Berlin, F.R. Germany.

By modifying the idea of the first algorithm of Remez for Chebyshev approximation problems, we can prove the convergence of a discretization method for the solution of nonlinear semi-infinite programming problems which only makes use of a relatively small finite subset of the infinite set of constraints in the program. We modify this algorithm further for linear problems and demonstrate its effectiveness in this case with a number of numerical examples. In particular, so-called singular problems are considered.

Stability of wide-angle absorbing boundary conditions for the wave equation.

R. A. Renaut, Arizona State University, USA.

Numerical stability of the two-dimensional wave equation requires mapping from a physical domain without boundaries to a computational domain with artificial boundaries. For realistic solutions, the artificial boundaries should cause waves to pass directly through and mimic total absorption of energy. An artificial boundary which propagates waves in one direction only is derived from approximations to the one-way wave equation and is commonly called an absorbing boundary. Here we investigate order two absorbing boundary conditions which include the standard Clayton and Engquist paraxial approximation.

Absorption properties are compared analytically and numerically. Our numerical results confirm that the L_∞ or Chebyshev-Pade approximations are best for wide angle absorption over a wide range of incident angles. Our results also demonstrate, however, that the boundary conditions are stable for varying Courant number. We prove that there is a stability barrier on the Courant number specified by the coefficients of the boundary conditions. In most cases this restriction is greater than that imposed by the stability of the interior scheme. Furthermore, waves may radiate spontaneously from the boundary causing instability, even if the stability bound on the Courant number is satisfied. Consequently, the Chebyshev and Least squares conditions may be preferred for wide angle absorption also.

Order results for Runge-Kutta methods applied to Differential Algebraic Equations.

M. Roche, Université de Genève, Switzerland.

Many problems in applications, e.g. constrained mechanical systems or simulation of electrical networks, lead to systems of differential equations given implicitly as

$F(Y, Y')=0$ with singular $\partial F/\partial Y'$. These systems, usually called differential algebraic equations (DAE's), often appear as differential equations together with certain constraints that the solution must satisfy, i.e. differential systems on manifolds.

The numerical solution of DAE's has been extensively studied in the last years. In this talk we shall study the order of convergence of Runge-Kutta methods applied to index 1 and 2 DAE's of the semi explicit form

$$y' = f(y, z), \quad 0 = g(y, z).$$

We shall show that some well known classes of Runge-Kutta methods are convergent of the same order as for non-stiff ordinary differential equations, whereas other methods suffer from a significant order reduction (index 2 case). Some results and conjectures about Runge-Kutta methods applied to index 3 systems will also be discussed.

Starting Methods for the Iteration of IRK's.

J. Sand, University of Copenhagen, Denmark.

In the application of an implicit Runge-Kutta formula (IRK) to a system of ordinary differential equations (ODE's), a substantial amount of work is spent in each step on solving the equations defining the internal stages. As these equations are solved by an iterative procedure, the accuracy of the starting values is essential and the usual starting methods have to be modified in order to treat stiff ODE's and/or large step-increases.

We show that an accurate starting method should be based on at least two different order of accuracy concepts: the conventional order and what we call the inverse order.

Existence and Linear Stability of Period 2 Solutions of Discrete Reaction-Diffusion Models with Various Types of Nonlinear Diffusion.

S. W. Schoombie, University of the Orange Free State, South Africa.

We consider the discrete model

$$U_j^{n+1} = U_j^n + \frac{\tau}{N+1} \left[(U_{j+1}^n)^{N+1} - 2(U_j^n)^{N+1} + (U_{j-1}^n)^{N+1} \right] + kU_j^n(1 - U_j^n).$$

In previous work the linear stability of period 2 solutions of this partial difference equation were considered for the cases $N=0$ and $N=1$. Here we discuss the existence and linear stability regions of similar period two solutions in the $k\tau$ plane for the cases $N=2$ and $N=3$. It is shown that in these cases the region of existence is the same as in the case $N=1$, but that the linear stability region corresponds more to that of the case $N=0$. It seems that the case $N=1$ may be rather special as far as these period two solutions are concerned.

Solving Large ODE Problems Using the Iterative Matrix Solver WATSIT

W. L. Seward, University of Waterloo, Canada.

Recently, interest has arisen in using iterative matrix solvers in codes for solving stiff ordinary differential equations (ODEs), motivated by a method-of-lines approach to time-dependent partial differential equations. The iterative methods of most promise are conjugate gradient and its variants. In this talk, I will describe an iterative solver package, WATSIT, developed at the University of Waterloo and its interface to the general-purpose ODE code, SPRINT.

Chan and Jackson (1986) gave an overview of the use of conjugate gradient-type methods in ODE codes and made some numerical investigations. They concluded that the methods were effective when used with preconditioning but that the choice of preconditioner needed further investigation. Brown and Hindmarsh (1986) investigated matrix-free iterative methods, in which storage of the Jacobian matrix is not required. The preconditioner used in WATSIT is a second-degree incomplete LU factorization which is more sophisticated than those tested by Chan and Jackson. Preliminary numerical tests indicate that it is robust and efficient. While it requires more storage than a matrix-free method, it is much cheaper than direct methods for large systems.

I will outline briefly the particular method used in WATSIT, and give some numerical results and comparisons to previous work. The convergence criteria used for the iterative method, which have a significant effect on performance, will be analysed. Numerical results indicate that the method is substantially more efficient than a direct solver on large sparse problems and is competitive on moderate-sized problems. The interface to the SPRINT package makes WATSIT as easy to use in the solution of ODE systems as any direct sparse solver.

Finite Element Approximation of a Model Reaction-Diffusion Problem with a Non-Lipschitz Nonlinearity.

R. M. Shanahan and J. W. Barrett, Imperial College, London.

Given $\lambda > 0$ and $p \in (0, 1)$, we consider the following problem

$$\begin{aligned} -\nabla^2 u + \lambda[u]_+^p &= 0 \quad \text{in } \Omega, \\ u &= 1 \quad \text{on } \partial\Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^2$ is a smooth convex domain. We prove optimal H^1 and L^∞ error bounds for the standard continuous piecewise linear Galerkin finite element approximation. In addition we analyse a more practical approximation using numerical integration on the nonlinear term. Finally, we consider a modified nonlinear SOR algorithm, which is shown to be globally convergent, for solving the algebraic system derived from the more practical approximation.

High order explicit Runge-Kutta pairs.

P. W. Sharp and E. Smart, University of Toronto, Canada.

Numerical testing over the last ten years has suggested explicit high order Runge-Kutta pairs are more efficient than VOMS Adams methods and low order pairs at most tolerances. In this talk we present new classes of high order pairs.

We begin with a brief review of the derivation of new and existing classes. Then we discuss the selection of coefficients from the classes and how the implementation of the pairs can differ from that of low order pairs. Finally, we present a summary of numerical comparisons between the new and existing classes.

Implementation of a Multigrid Method on a Transputer Network.

G. J. Shaw and A. Stewart, University of Oxford and Queen's University, Belfast.

The multigrid has become widely accepted as the most efficient process for the solution of elliptic partial differential equations. The result of applying a few iterations of some classical relaxation method is that the error becomes smooth. The multigrid approach recognises that once an error is smooth its residual equation may be represented accurately on a coarser grid, where its solution is easier. By applying this

principle recursively on a sequence of grids of differing steplengths we arrive at a method which reduces all types of error equally efficiently and therefore has optimal convergence properties.

In this paper we present an implementation of the multigrid algorithm on a 32 processor transputer network. Our aim in this work is that the multigrid method should maintain the parallel efficiency of the underlying smoothing method, whilst achieving vastly improved convergence rates.

Results are presented for the solution of Poisson's equation by a multigrid method using Red-Black Gauss-Seidel as a smoother. On a typical 128×128 grid the results are as follows. The parallel speed up for Red-Black in its own right is 25. The corresponding speed up for Red-Black with multigrid is 20. The overall speed up for parallel multigrid over serial Red-Black approaches a factor of 10000.

Work is currently in progress to extend the method to more complicated problems, including solution of the Euler equations for transonic flow.

The Global Error Estimate of Exponential Splitting.

Q. Sheng, University of Cambridge, U.K.

Various kinds of the exponential splitting methods are used nowadays to compute the numerical solutions of partial differential equations. It may be extremely important to give the necessary error estimates to different splitting schemes. Much effort has been devoted during recent years to the local error analysis. However, it is found that the local truncation errors are not adequate to describe the error behaviour of the exponential splitting schemes. In this paper, we provide the global error analysis to the principal splitting techniques and global estimates are obtained. The investigations are also given when the linearly perturbed error relations are introduced.

Some Observations on the Streamline Upwind Petrov Galerkin Method for Convection-Diffusion Problems.

S. Sigurdsson, University of Iceland.

The Streamline Upwind Petrov Galerkin (SUPG) method for the solution of convection-diffusion problems, introduced in its first form by Hughes and Brooks ten years ago and subsequently analysed by Johnson and his co-workers, has been shown to possess valuable stability properties without suffering undue loss in accuracy. We shall seek to relate this method to some other proposed modifications of the Galerkin finite element method, in particular the idea of choosing as test functions within the elements the solutions of appropriate adjoint problems. Our contention is that this provides a useful guidance in choosing the values of the free parameters in the SUPG method as well as in extending it to more general problems. The emphasis is on two-dimensional problems where linear or quadratic basis functions on triangular elements are used.

Conjugate Gradient Algorithms for Stabilised Mixed Finite Element Methods.

D. J. Silvester and N. Kechkar, UMIST, U.K.

At the 1987 Dundee conference, theoretical results pertaining to the development of new classes of mixed finite element methods were presented by Hughes and Franca. Within the framework of incompressible flow modelling based on discontinuous pressure approximation, these new methods achieve universal stability by augmenting the discrete incompressibility constraints by inter-element pressure jump terms. A mixed method which is stabilised in such a way is referred to here as a global jump

formulation. Our recent work (in Numerical Analysis Report 165, University of Manchester/UMIST Joint Series), has demonstrated that a more effective stabilisation of low-order mixed methods can be achieved using analogous local jump formulations. The principal advantage of such a local approach is that the resulting mixed method is considerably more robust with respect to the magnitude of the stability parameter. In addition, when using a local stability framework implementation into existing flow codes is significantly easier.

The primary motivation for stabilisation is the fact that improved stability increases the potential for fast iterative solution using multigrid, or preconditioned conjugate gradient algorithms. The talk will focus on the necessity of ensuring stability if fast solution of incompressible flow problems is to be achieved. To illustrate the general benefit that arises from increased stability, the performance of different conjugate gradient algorithms from the NSPCG package (Oppe, Joubert and Kincaid, Report CNA-216, University of Texas at Austin) will be compared for the solution of a standard test flow problem. The emphasis will be on assessing the relative efficiency of these algorithms in a vector processor environment.

Accurate Fourier pseudospectral solution of the RLW equation
D. M. Sloan, University of Strathclyde, UK.

Peregrine proposed the regularised long wave (RLW) equation as an alternative to the KdV equation for the propagation of certain kinds of water waves. Olver has shown that the RLW equation has only three solution invariants. A pseudospectral method is discussed which, in semi-discrete form, satisfies two of the invariance conditions. Stability and accuracy of the scheme are considered. Numerical results show the fine structure of inelastic soliton collisions and the interaction of nearly-equal solitons.

Block Runge-Kutta Methods on Parallel Computers.
B. P. Sommeijer, CWI, Amsterdam.

In solving the initial value problem $dy(t)/dt = f(y(t))$, $y(0) = y_0$ by means of a block method, one step of such an algorithm yields a number of approximations to the solution at different points t_n .

By properly choosing the parameters in such methods, this number of approximations can be computed concurrently, thus exploiting the features of a parallel computer architecture. Most of the parallel block methods proposed in the literature are based on the concept of linear multistep methods (cf.e.g. [1] and [2], i.e. the points t_n are equally spaced.

In this talk we show what can be obtained if we allow the simultaneously produced approximations to correspond to nonequidistant points, a situation similar to the intermediate approximations computed in Runge-Kutta methods [3].

This approach enables us to improve the order of accuracy. Examples will be presented of methods up to order 8, suitable to be used on 2-processor machines and requiring (effectively) 2 evaluations of the derivative function f per step.

This work was jointly done with P. J. van der Houwen.

[1] P. B. Worland, Parallel methods for the numerical solution of ordinary differential equations, IEEE Trans. Comput. C-25, 1045-1048(1976). [2] M. T. Chu & H. Hamilton, Parallel solution of ODEs by multi-block methods, SIAM J. Sci. Stat. Comput. 3, 342-353(1987). [3] P. J. van der Houwen & B. P. Sommeijer, Block Runge-Kutta methods on parallel computers, Report NM-R8906, Centre for Mathematics and Computer Science, Amsterdam, The Netherlands(1989).

Optimal Lattice rules in Dimension 2 and 3.

T. Sorevik and J. N. Lyness, University of Bergen, Norway and Argonne National Laboratory, U.S.A.

Lattice rules are quadrature rules for the unit hypercube, first introduced by Sloan and Kachoyan (1984,1987). They are generalisation of the well known number theoretic rules of Korobov (1959).

The quality of lattice rules are usually measured by the Zaremba-index. Finding optimal number-theoretic rules, in terms of highest Zaremba-index for given dimension and number of abscissas, has been in the focus of interest for many researcher. Only in dimension 2 closed form solutions to the problem has been found. We have extended this solution to include all 2-d lattice rules.

For higher dimension no closed form solutions are known, leaving us with extensive computer searches for finding the optimal lattice. For fixed dimension there is a large number of lattice rules of given order. Thus the task of searching through every lattice rule, computing its Zaremba-index and finding the best is computational very heavy. We will discuss how to take advantage of the theory of lattice rules to speed up the computation and present results for the 2 and 3 dimensional case.

Ill - posedness and singular integrals in the boundary integral method.

Jacob Steinberg, Technion - Israel Institute of Technology.

We consider a model problem of fracture mechanics and the series expansion of its solution around the singular point, Williams' series. A boundary integral representation of the coefficients involves given boundary conditions as well as unknown values for which a pair of integral equations must be solved. This is an ill-posed problem leading to an ill-conditioned matrix in any numerical treatment. It is shown how the analytic continuation of biharmonic functions is used in order to reduce the condition number. However many singular integrals appear; they can be expressed by means of seven standard types.

Spurious Dynamics in Numerical Simulations of Differential Equations.

A. Stuart, University of Bath, U.K.

We compare the dynamics of time-dependent differential equations and their discrete analogues. Our approach is to consider the time-step Δt as a bifurcation parameter and to identify the critical values of Δt at which the dynamics of the discretisation undergo qualitative changes. Using small amplitude bifurcation theory we prove the result that linearised numerical instability implies spurious dynamics. A large norm theory is also developed to analyse the possibility of spurious dynamics when the numerical method is operating well below its linear stability limit (i.e. as $\Delta t \rightarrow 0$.) Several illustrative examples from ODE theory are presented and the approach is then applied to a general class of reaction-diffusion-convection equations.

Spectral Transport-diffusion Algorithm for Convection-diffusion Problems.

E. Süli and A. Ware, University of Oxford, U.K.

We introduce a new numerical technique for convection-dominated diffusion problems, based on combining a spectral spatial discretization with timestepping along characteristics, which permits the use of large time steps at no cost in accuracy. The method is shown to be unconditionally stable and spectrally accurate. The theoretical results are illustrated with numerical experiments.

Numerical solution of retarded ode-systems.

P. G. Thomsen, Technical University of Denmark.

In modelling the motion of ships one deals with systems of ODE's that have retardation terms in the form of convolution integrals. The dimension of the system corresponds to the number of degrees of freedom for the dynamic system. In special cases the dynamic system may have the characteristics of a stiff system of ode's and the choice of numerical method must be done accordingly.

The numerical solution method that is described is based on SDIRK methods and the convolution terms are computed by numerical quadrature or FFT. The implementation of the solution method on a network of transputers will be discussed. Numerical examples are discussed.

The Finite-element Method with Nodes Moving along the Characteristics for Convection-Diffusion Equations.

Y. Tourigny, and E. Süli, University of Oxford, U.K.

We examine the convergence properties of the finite-element method with nodes moving along the characteristics for one-dimensional scalar convection-diffusion equations. For linear elements, we show

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + \sqrt{\epsilon} \|u_h(t) - u(t)\|_{L^\infty(\Omega)} = O(h^2)$$

where the underlying constant depends on the diffusion coefficient ϵ only through (some Sobolev norm of) the solution u . The result holds for both linear and nonlinear problems. In the latter case, however, we have to assume that mesh tangling does not occur. Numerical results are presented.

Polynomial higher order predictors in numerical path following schemes.

Klaus Ulrich, University of Hannover.

A class of polynomial higher order predictors for numerical path following schemes is presented which can be interpreted via reduced basis methods. Information gained from these terms can even be used for sensitivity analysis purposes.

Explicit computation of first order derivatives only is required, no process of numerical differentiation is involved to obtain the additional higher order terms. Information gained from these terms can even be used for sensitivity analysis purposes.

The new predictor method presented here offers a variety of advantages and possible applications.

The method is hierarchical and adaptive; predictors of varying order may be used on following a solution curve; the method is robust: the quality of prediction does not change much with moderate changes of the locations of the base points, nor with the ordering of these points; the method allows to detect the possible presence of limit points without having to compute solution points beyond such points; the method allows to monitor the approximation quality by means of a forward-backward strategy.

A shape preserving curve interpolation scheme using parametric rational cubic splines.

K. Unsworth, and T.N.T. Goodman, University of Dundee.

A local convexity preserving parametric interpolation scheme is described using piecewise rational cubics. The scheme requires a tangent direction and curvature value to be assigned at each interpolation point. One method of choosing these values is described

in order to reproduce circular arcs. It is shown that this scheme has all of the desirable properties possessed by earlier schemes proposed by the authors, and in addition offers a number of further advantages. Illustrative examples will be given.

The Difference Interpolation Method for Splines.
W. Volk, Berlin, F.R. Germany.

The difference interpolation method (DIM) was first introduced for the evaluation of univariate polynomials at many equidistant points of the real line (Volk, 1988). The DIM is a typical raster evaluation method, which means that it uses the fact that each point has constant distance to its neighbours. This method uses also some relations between forward differences associated to different step sizes. They are of independent interest.

This method was also applied to spline functions by Volk (1989). The aim of the lecture is now to introduce some modifications to the method. There are some close connections to combinatorics. Due to some abstract relations in this field, a more stable procedure is achieved. Moreover some computational inadequacies are avoided. By numerical examples it will be demonstrated that there is no significant lack of precision, but depending on some circumstances a really faster runtime of the algorithm.

Finite Element Computation on Multiprocessor computer.
R. Wait and C. J. Willis, University of Liverpool, U.K.

In view of the size and structure of the problem, finite element analysis is a promising candidate for implementation on a distributed architecture machine. The generation of the element matrices is an example of what has been termed "embarrassingly obvious parallelism" as, in a typical large scale engineering analysis, there are hundreds of similar (possibly identical) disjoint tasks that involve no communication. The global assembly involves local (ie short range) communication and this has led to a predominance of implementations based on domain decomposition (ie geometric parallelism).

With time dependent problems for which an explicit (ie lumped) time stepping formulation is possible, the interprocessor communication (ie interdomain) connectivity in the solution algorithm involves the same local communication as for the global assembly. Hence there is a consistent criterion for a "good" domain decomposition in terms of size and surface/volume ratio of the subdomains.

Domain decomposition using optimisation techniques based on simulated annealing and on neural network models have both been suggested, but these approaches appear to be very computer intensive. We give examples of the use of a simpler algorithm based on the ideas used in mesh ordering for bandwidth (or frontwidth) minimisation.

For equilibrium problems, there is a global interdependence of the solution and the f.e. analysis involves the solution of a set of simultaneous algebraic equations. The objective function in the domain decomposition optimisation is now dependent on the solution algorithm. It has to include some measure of the computational complexity of the solution relative to the communication cost. The simple ordering strategy does not take explicit account of the computational cost and hence it is still valid, although not necessarily particularly effective.

We give examples of different solution algorithms and discuss the relative efficiencies of the methods with reference to our numerical experiments on transputer arrays.

The Use of the Basic Linear Algebra Subprograms (BLAS) in improving supercomputer speeds.

Jerzy Wasniewski, The Danish Computer Centre for Research and Education.

The multiprocessing computers, vector and parallel, are much more difficult to program than the conventional scalar machines. The program is written (we assume all the algorithm operations are performed in the core) in the standard portable computer language, for example Fortran 77 and usually runs with the computer peak performance speed on every scalar computer. This program, of course, runs correctly on a supercomputer too. If it has no special machine dependent preparation its speed is very far from the top speed performance. To achieve good supercomputer speed one needs to use special machine dependent programming techniques.

The compilers will probably solve the above mentioned problems in the future. For the present the standard Basic Linear Algebra Subprograms (BLAS) are specified. Three BLAS levels are defined: BLAS level 1 for vector-vector operations, BLAS level 2 for matrix-vector operations and BLAS level 3 for matrix-matrix operations. The BLAS should be specialized for each computer (supercomputer). They use all the machine specific properties, e.g., vector processing, multiprocessing, cache memory, and so on. They can be written either in machine language or in Fortran, using the machine properties by the compiler directives and special compiler machine dependent innovations.

Therefore, an algorithm written in standard Fortran 77 language calling the BLAS for the basic linear algebra operations will perform efficiently on each computer (supercomputer).

As an example, the Amdahl Vector Processors (VP) BLAS will be explained. The presentation will describe various techniques for improving the computational speed of the Level 2 BLAS on Amdahl vector processors. Performance measurements will be given which demonstrate the improvements obtained, for the Level 2 BLAS themselves and for linear algebra routines which call them.

Optimal Grids and Solutions for Compressible Flows in Nozzles.

J. Wixcey, University of Reading, U.K.

For quasi-one-dimensional adiabatic and shocked flow in a nozzle there exist well-defined relationships between the flow variables which may be used to generate an exact solution. Stationary principles equivalent to the equations governing the flow are described and used to determine an approximate finite element solution for the axial fluid speed on an adaptive grid, in which the solution for the axial fluid speed and an optimal finite element grid are obtained simultaneously.

Hopscotch for Parabolic PDEs.

A. S. Wood, University of Bradford, U.K.

In this talk a critical assessment of the hopscotch finite-difference algorithm (as applied to linear diffusion-like problems) is presented.

The basic odd-even algorithm as formalised by Gourlay [1] will be explained. Two one-dimensional test problems with smooth/step-like initial conditions will be used to illustrate the properties of hopscotch in relation to the well-known explicit, implicit and Crank-Nicolson schemes. Stability, truncation error (convergence), the behaviour of errors and coding considerations will be presented for these schemes, the aim being to show that hopscotch is an under-valued (and under-used) numerical process.

[1] A. R. Gourlay, Hopscotch: A fast second-order partial differential equation solver, JIMA, 6, 375-390 (1970).

A Parallel Algorithm for Banded Linear Systems.

S. J. Wright, Argonne National Laboratory, U.S.A.

A partitioned Gaussian elimination algorithm with partial pivoting which is suitable for multiprocessors with small to moderate numbers of processing elements is described. We only assume that the system is non-singular; hence the submatrices in our chosen partitioning may be rank-deficient and this makes the algorithm more complex than those which have been proposed for diagonal-dominant and symmetric positive definite systems. The effect of ill-conditioning in these sub-matrices on the solution accuracy is examined. We discuss application of these techniques to problems in discrete-time optimal control, and present some numerical results obtained on Alliant, Sequent and Encore multi- processors.

A Moving-Grid Interface for Systems of One-Dimensional Time-Dependent Partial Differential Equations.

P. A. Zegeling, and J. G. Blom, CWI, Amsterdam.

In the last decade several numerical techniques have been developed to solve time-dependent Partial Differential Equations (PDEs) in one dimension having solutions with steep gradients in space and in time. One of these techniques, a moving-grid method based on a Lagrangian description of the PDE and a smoothed-equidistribution principle to define the grid positions at each time-level, has been coupled to a spatial discretization method which automatically discretizes the spatial part of the user-defined PDE following the Method of Lines approach. We supply two subroutines, CWRESU and CWRESX, which compute the residuals of the ODE system obtained from semi-discretizing resp., the PDE and the set of moving-grid equations. These routines are combined in an enveloping routine SKMRES which delivers the residuals of the complete ODE system to be used in a SPRINT environment. To solve this stiff, nonlinear implicit ODE system, a robust and efficient time-integrator must be applied, such as one of the BDF modules in SPRINT. Some numerical examples are shown to illustrate the simple and effective use of this software interface.

Properties of the approximations of a matrix which lower its rank.

K. Ziętak, University of Wrocław, Poland.

Let C be a real $(m \times n)$ -matrix. One considers the general properties of the best approximations E to C in an arbitrary norm by matrices of rank $\leq r$. Separately, one deals with the case in which $\text{rank } C = n$, $r = n-1$ and $\|\cdot\|$ is a separable norm. For this particular case the form of every best approximation E and an estimation of the error $\|C - E\|$ are given. One also investigates when for this particular case the best approximation E is unique.