

DUNDEE BIENNIAL CONFERENCE ON NUMERICAL ANALYSIS

UNIVERSITY OF DUNDEE

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ABSTRACTS

Section A Invited talks

Section B Submitted talks

SECTION A

On the Dimension of Multivariate Piecewise Polynomials

P Alfeld, University of Utah, U.S.A.

Lower bounds are given on the dimension of piecewise polynomial C^1 and C^2 functions defined on a tessellation of a polyhedral domain into Tetrahedra. The analysis technique consists of embedding the space of interest into a larger space with a simpler structure, and then making appropriate adjustments. In the bivariate case, this approach reproduces the well-known lower bounds derived by Schumaker.

An Algebraic Condition for A-stable Runge-Kutta Methods

G J Cooper, University of Sussex.

The concept of A-stability for Runge-Kutta methods is examined and an algebraic condition is obtained. A corresponding concept, for a system of linear autonomous differential equations, yields a simpler algebraic condition. This condition is a generalization of the algebraic condition for B-stability.

Strategies for Constraint Deletion in Active Set Algorithms

D Goldfarb, Columbia University, U.S.A.

We give strategies for simultaneously dropping more than one constraint from an active set which ensure that the step taken after these constraints are dropped is along a feasible direction. Various criteria for choosing a particular constraint to drop when there are several candidates are discussed. We also show how our strategies can be implemented efficiently.

Optimization via Quasi-Newton Updated Conjugate Subspaces

Shih-Ping Han, University of Illinois, U.S.A.

Based on the close relationship between the quasi-Newton method and the conjugate direction method, we develop a class of methods which are particularly suitable for parallel computation. In each iteration of these methods, the R^n space is decomposed into several subspaces which are conjugate with each other with respect to an underlying estimate of a Hessian. Minimization of the given functions over each subspace is carried out independently to produce a new estimate of a solution. The conjugate subspaces can be updated by a quasi-Newton scheme. By so doing, the resulting methods possess all the nice convergence properties a quasi-Newton method has. Moreover, this approach provides a unified view of the quasi-Newton method, the conjugate direction method and the pattern search method.

Order Stars and Stability Barriers
A Iserles, University of Cambridge.

Barriers on order for stable numerical methods for differential equations of evolution have been known since the pioneering work of Dahlquist. The subject received new impetus with the introduction of order stars by Wanner, Hairer and Nørsett in 1978. In the present talk we will use order stars to derive stability barriers for a whole spectrum of problems: one-step multi-stage linear methods for $y' = f(t, y)$, one-level and multi-level discretization of $u_t = u_x$, one-level methods for $u_t = u_{xx}$, as well as generalizations of the original Dahlquist barriers.

Parallel Algorithms for Constrained and Unconstrained Least Squares Problems
C Van Loan, Cornell University, U.S.A.

The minimization of $\|W(Ax - b)\|_2$ subject to the constraint $s^T x = 1$ is a problem of considerable importance in certain real-time signal processing settings. Here, $W \in \mathbb{R}^{m \times m}$ is a highly structured weighting matrix, $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, and $s \in \mathbb{R}^n$. For a given A , one must typically solve this problem for many different constraint vectors s . In addition, A itself is periodically updated. We'll discuss an algorithm for solving this problem that has a significant amount of parallelism.

Numerical Calculations of Isolated Coherent Spots in a Turbulent Two-Dimensional Flow
P S Marcus, Harvard University, U.S.A.

We present the results of numerical calculations for nearly two dimensional (quasi-geostrophic) flow in a rapidly rotating, short aspect-ratio annulus with a sloping bottom boundary. Both viscous and inviscid flows were examined and a variety of geometries (including those with no inner radial boundary) were studied. Calculations were performed using pseudo-spectral and spectral (i.e. no aliasing error) methods, as well as with point-vortex, finite-core vortex, and vortex-in-cell methods so that the numerical techniques could be compared with respect to accuracy and efficiency. The flow itself is of interest because we find that for a wide variety of initial conditions, the flow settles into a statistically steady state that consists of one (and only one) isolated spot of vorticity surrounded by a chaotic flow. The numerical results have lead to an analytic model of this turbulent flow. Our model explains many of the flow's features and also helps to explain the different problems associated with each of the numerical methods that we used in calculating this flow numerically. We note that an inviscid two-dimensional flow has an infinite number of conserved quantities, and by using statistical mechanics we show why only some of these quantities are important in determining the large-scale structure of the equilibrium flow and why others are unimportant. We show that the differences among the numerical methods that we used are due in part to their treatments of the conserved quantities.

Beyond the Linearised Stability Limit in Nonlinear Problems

A R Mitchell*; D F Griffiths, University of Dundee.

In recent years the computer has greatly augmented the understanding of nonlinear processes. The most exciting developments, however, have come not from numerical analysts, but from physicists, biologists, etc. equipped with a small computer, and solving nonlinear difference equations.

In the present talk, two widely different examples of recent developments in the analysis of nonlinear problems are given

(i) The apparently chaotic behaviour of deterministic dynamical systems with parameters and their relation with standard time stepping procedures in ordinary and partial differential equations. These "new" solutions, involving bifurcation, period doubling, chaos etc. emerge from step lengths in time beyond those allowed by the von Neumann linear stability criterion.

(ii) Nonlinear dispersive wave problems and the emergence of soliton solutions from instabilities introduced by the initial data. Again the partial difference approximations are operating beyond the linearised von Neumann limits. The equations considered are the Nonlinear Schrödinger and Korteweg de Vries equations.

On Characteristic Galerkin and Lagrange Galerkin Methods

K W Morton, Oxford University Computing Laboratory.

The idea of combining the Galerkin projection with following the characteristics or the material derivatives has proved very fruitful in a number of applications areas - e.g. diffusion-convection, Navier-Stokes, shock modelling in compressible flow.

We shall discuss various alternative formulations which have been used and the importance of devising appropriate quadrature rules if the attractive stability and accuracy properties of the underlying methods are not to be unacceptably degraded.

New algorithms have recently been developed, based on piecewise constant elements but supplemented by adaptive recovery techniques using piecewise linears, to give second order accuracy and monotonicity preservation for hyperbolic conservation laws. We shall consider the problems of extending these algorithms from their present one-dimensional form to genuinely two-dimensional forms.

Numerical Methods for Solving Matrix Inverse Eigenvalue Problems
M L Overton, Courant Institute of Mathematical Sciences, U.S.A.

Consider the following problem: given real symmetric $n \times n$ matrices $\{A_k\}$, $k=0, \dots, n$, find real parameters $\{c_k\}$, $k=1, \dots, n$, such that

$$A(c) \equiv A_0 + c_1 A_1 + \dots + c_n A_n$$

has given eigenvalues $\lambda_1^* \geq \dots \geq \lambda_n^*$. Variations of this model problem, often associated with a minimization process, arise in many different application areas, including nuclear spectroscopy, Sturm-Liouville problems, control theory, structural analysis, graph partitioning and rank minimization problems. The model problem may be formulated in several ways as a system of nonlinear equations. This leads to the consideration of several different numerical methods to solve the problem, all connected in some way with Newton's method. Some of these methods, such as those due to Downing and Householder, Kublanovskaja, and Biegler-Konig, require computation of eigenvalues and eigenvectors at each step of an iteration. Two other methods, one due to Osborne and one apparently new, do not require computing eigenvalues. We are particularly interested in the case where the $\{\lambda_i^*\}$ include multiple eigenvalues. In this case the eigenvectors are generally not continuous functions of the parameters $\{c_k\}$ and the nonlinear systems generally become nondifferentiable. Nonetheless, we show how the problem formulations should be modified in the multiple eigenvalue case to give numerical methods which are quadratically convergent. We illustrate the results by numerical experiments. This work is joint with Stmuel Friedand and Jorge Nocedal.

Global Optimization Methods

A H G Rinnooy Kan, Erasmus University, Rotterdam.

We shall provide a brief survey of methods for global optimization of a smooth objective function. The emphasis will be on methods that involve a mixture of sampling, clustering and local search techniques. They combine strong theoretical properties with attractive computational behaviour.

Nonlinear Instability: the Dynamic Approach

J M Sanz-Serna*; F Vellido, Universidad de Valladolid, Spain.

It is well known that, when Δt is fixed and t increases, the qualitative behaviour of numerical approximations to solutions of evolutionary differential equations is likely to be widely different from that of the theoretical solution. A typical instance is given by the so-called nonlinear instability, first discovered by Phillips: the computation blows up even if the theoretical solution remains bounded and sufficient conditions for linear stability are satisfied. Recently, there has been interest in investigating this sort of phenomena from the point of view of the theory of dynamical systems. In the talk we will demonstrate the application of this technique by means of an example which fully illustrates the powerful insights that can be derived from the dynamic approach.

Dispersion, Dissipation, and Stability

L N Trefethen, Massachusetts Institute of Technology, U.S.A.

Dissipation in finite difference models can be quantified by considering amplification factors, and dispersion by considering group velocities. Since the latter analysis is not so common, this talk will first review group velocity effects in numerical computation. Then it will be shown that in several contexts, dispersion is not only of behavioral importance, but is the mechanism of instability.

Convergence and Order Reduction of Diagonally Implicit Runge-Kutta Schemes in the Method of Lines

J G Verwer, Centre for Mathematics and Computer Science, Amsterdam.

We examine four known diagonally implicit Runge-Kutta discretizations of initial-boundary value problems in partial differential equations. Our main interest lies in the derivation of bounds for the full discretization error under the assumption that the grid distance in space and time are independent parameters. We follow the method of lines approach which enables us to exploit ideas and results from the B-convergence theory for Runge-Kutta schemes applied to stiff problems. Emphasis is laid upon order reduction phenomena. Various numerical examples are presented which illustrate and confirm the theoretical results. It is shown that in the field of partial differential equations order reduction frequently occurs and severely reduces the performances of high order Runge-Kutta schemes.

Splines versus trigonometric polynomials - the h versus the p - version in two-dimensional boundary integral methods

W L Wendland, Technische Hochschule Darmstadt, Germany

The different choices of trial functions for the approximation of the boundary data of two-dimensional elliptic boundary value problems lead to different boundary element methods. Here we present spline Galerkin and spline collocation (the h-version) and Fourier series (the p-version) approximations of the boundary integral equations together with corresponding asymptotic error estimates.

SECTION B

The Implementation of Hybrid Formulae for Initial Value Differential Equations

C A Addison, University of Alberta, Canada.

We examine some of the details involved in an efficient implementation of the hybrid formulae derived by England for stiff initial value differential equations. A member of this family of formulae is obtained by combining a variation of an Adams Moulton formula that employs an off-step point with a variation of a backward differentiation formula that is used to give an approximation to the solution at this off-step point. The formulae all have good accuracy and stability properties which make them well suited for a code intended to solve both stiff and non-stiff problems.

The specific issues discussed include the choice of representation, the solution of the nonlinear equations that arise on each step, the choice of the predictor and the use of these formulae on linear, constant coefficient problems. The results obtained from a preliminary code using these formulae are contrasted with the results obtained from other codes. These results are then used to motivate future work that needs to be done.

A boundary integral technique for the calculation of immiscible flow in a porous medium

J M Aitchison, Royal Military College of Science.

We consider the classical two-dimensional Muskat problem in which one fluid (Fluid I) is injected into a porous medium through a point source at point A and displaces a second fluid (Fluid II) which leaves through a point sink at point B. Let R_1 denote the finite region occupied by fluid I, R_2 the infinite region occupied by fluid II and let C be the interface between them (assumed sharp). Our major interest is in the movement of the interface C with time - in particular how long it takes to reach B. However this can only be calculated by solving, at each time step, an elliptic partial differential equation in each of the regions R_1 and R_2 - these equations being linked through the boundary conditions on C.

Such a problem is well-suited to a boundary integral approach, and has several features which would make a solution by standard numerical techniques difficult. In particular we will show how the boundary integral method can deal with the infinite region R_2 , with the point source and sink, and with the coupling of the equations in the two regions. The problem is then reduced to one of tracking the interface C through time, which will also be discussed.

Optimal Variable Metric Methods for Unconstrained Optimization
M Al-Baali, University of Damascus, Syria.

In this talk, I show that the well known Broyden updating formula (which contains a parameter, θ say) solves two scalar measures subject to certain conditions. One of those measure defines the change to certain current Hessian approximation, and the other is the change to certain current inverse Hessian approximation. Minimizing such a combination of both measures with respect to the parameter θ leads to define this parameter in an optimal way, for which an optimal updating formula, for unconstrained optimization is obtained.

Other interesting results are also presented.

Rigorous error bounds for singular values of a matrix using the precise scalar product
G Alefeld, University of Karlsruhe, Germany.

Let there be given a real approximation σ to a simple singular value and real vectors $u \in \mathbb{R}^n$ and $v \in \mathbb{R}^m$ as approximations to the right and left singular vectors of a real (m,n) matrix A . Then we consider the problem of computing rigorous error bounds for these approximations.

We present a nonlinear system consisting of $m+n+2$ equations and $m+n+2$ unknowns whose solution delivers an exact singular value and the exact components of the right and left singular vectors belonging to this singular value.

We then show that for sufficiently accurate approximations we can compute intervals in which the unknowns are located.

Starting with these inclusions we present an iterative method which improves these intervals repeatedly and which is convergent to the exact values if no rounding errors are involved.

Finally we perform a detailed analysis of the proposed method if it is performed on a computer using a floating point system. For this discussion we assume that the so-called precise scalar product introduced by U. Kulisch is available.

Some numerical examples are presented.

Finite Element Analysis of Bifurcation of Thin, Shallow, Spherical Shells

P J Aston ; J R Whiteman , Brunel University.

Marguerre's shallow shell equations are used to describe the deformation of the shell in terms of the vertical displacement w and a stress function F . Reissner's mixed variational principle is used to represent these equations. Bifurcation from the axisymmetric path is analysed by considering small asymmetric deviations of the form

$$w(x, \theta) = \sum_{n=1}^{\infty} w_n \cos n\theta .$$

Bifurcation points are found for each value of n separately by considering an extended system. As the extended system finds the bifurcation point directly continuation methods can then be used to follow bifurcation points for varying shell parameters.

Results are presented for bifurcations of the shell both snapping and snapping back for clamped and simply supported boundary conditions.

The Simple Quadratic Penalty Function and the S.Q.P. Methods

N F Attia*; C G Broyden, University of Essex.

For many years, the simple quadratic penalty function methods have been regarded as inefficient methods of solving the nonlinearly constrained optimization problems. We present a numerically reliable algorithm which utilizes such methods combined with an orthogonal transformation derived from the Jacobian of the constraints. The relationship with the S.Q.P. methods is outlined and encouraging numerical results are presented.

Quadratic Parametric Transformations

M L Baart, NRIMS, Pretoria, South Africa.

Techniques used in finite element methods to approximate two-dimensional regions with curved boundaries are eminently suitable for application to computer aided design. One such technique involves the parametric transformation of polygonal master-elements. When combined, the images of the elements should form a bijective image of the original straight-edged domain, and the image domain is used to approximate the required curved domain. We shall consider various aspects of the bijectivity of quadratic parametric transformations of convex polygonal master-elements.

The theorem that usually provides sufficient conditions for the global bijectivity of a transformation is that of De la Vallée Poussin. We show that the conditions can be relaxed slightly for all quadratic parametric transformations. The non-vanishing of the Jacobian over a convex master-element is namely a sufficient condition to ensure bijectivity, while it is necessary for an injection that the Jacobian does not vanish in the interior of the element.

Properties of the Jacobian of the general quadratic parametric transformation are now used to construct a simple and efficient algorithm to check for vanishing Jacobians and thus to ensure bijectivity. The sign of the Jacobian at all the master-element vertices must be the same. For nonlinear Jacobians we check for Jacobian zeros on the edge segments, and for elliptic Jacobians we also have to check that any one point where the Jacobian is zero, is outside the master-element.

For those quadratic transformations that result in linear Jacobians we derive a connection between bijectivity and overspill. The image of the line on which the Jacobian vanishes is namely the boundary of the image domain of the plane, except in special cases where the line is mapped onto a single point.

As an application we consider quadratic parametric transformations of triangles with fixed vertices and perturbed side midpoints, and discuss several examples.

Local Moving Finite Elements

M J Baines, University of Reading.

The Moving Finite Element method, introduced by Miller in 1981, is described and shown to be a local method, at least in one dimension, which gives the evolution of each linear segment of the solution separately. As a result, non-linear scalar partial differential equations in one dimension (with or without shocks) can be solved easily on a microcomputer.

The local property of the method in two dimensions is discussed and a variant of the MFE method proposed which involves only inversion of 3×3 matrices. Extensions to systems are also described.

Finite Element Approximation of the Dirichlet Problem using the Boundary Penalty Method

J W Barrett*; C M Elliott, Imperial College.

This paper considers a finite element approximation of the Dirichlet problem for a second order self-adjoint elliptic equation, $Au = f$, in a region $\Omega \subset \mathbb{R}^n$ ($n = 2$ or 3) by a boundary penalty method. If the finite element space defined over D^h , a union of elements, has approximation power h^K in the L^2 norm, then

(i) for $\Omega \in D^h$ convex polygonal, we show that choosing the penalty parameter $\varepsilon \equiv h^\lambda$ with $\lambda \geq K$ yields optimal H^1 and L^2 error bounds if $u \in H^{K+1}(\Omega)$.

(ii) for $\partial\Omega$ a smooth curve, an unfitted mesh ($\Omega \in D^h$) and assuming $u \in H^{K+1}(\Omega)$ we improve on the error bounds given by Babuska (1973). As (ii) is not practical we analyse a fully practical piecewise linear approximation involving domain perturbation and numerical integration. We show that the choice $\lambda = 2$ yields an optimal H^1 and interior L^2 rate of convergence for the error. A numerical example is presented confirming this analysis. Finally, we apply the technique and analysis to the interface problem.

An Exact Penalty Method for Solving Nonlinearly Constrained Nonlinear Least Squares Problems

R H Bartels; N Mahdavi-Amiri*; York University, Canada.

The penalty method for solving constrained nonlinear programming problems as proposed by Coleman and Conn is adapted to solve constrained nonlinear least squares problems. The adaptation takes into consideration the special structure of the objective function and extends the quasi-Newton strategies in the unconstrained case to the constrained in computing an update for the Hessian of the penalty function in successive iterations. A computer implementation of our algorithm is discussed along with test results obtained in the course of algorithm development.

Finite Element Treatment of Singularities in Elliptic Problems Using Non-exact Augmentation

A E Beagles; J R Whiteman, Brunel University.

When solving elliptic boundary value problems containing boundary singularities using finite element methods, the benefits of augmenting the trial and test function spaces with functions appropriate to the forms of the singularities are well known. However, for many problems it is not possible to calculate the appropriate singular functions exactly. Examples of this are two-dimensional Poisson interface problems and three-dimensional Poisson problems with re-entrant vertices.

For such problems, methods of obtaining the approximate forms of the singularities are presented and it is demonstrated how, in the finite element method, the benefits of augmenting the test and trial function spaces with exact singular functions can be obtained using augmentation with non-exact functions.

Stability Properties for Continuous Extensions of Discrete ODE Methods

A Bellen; M Zennaro, University of Trieste, Italy.

In solving IVP's for ODE's we need often know the solution on a set of points also other than the grid points (systems with driving equations, dense output, discontinuity problems, delay equations...).

Different conditions can be imposed to the continuous extension, according to the nature of the problem we deal with. In particular, we investigate whether the continuous extension maintains the stability properties of the discrete method. In other words we analyze how to avoid high oscillations in the continuous extension, which make the global approximation unacceptable, as it may possibly happen, for example, in solving stiff equations.

Numerical Stability of the Method of "Semi-Normal Equations" for Solving Least Squares Problems

Å Björck, Linköping University, Sweden.

The least squares problem $\min_x \|Ax - b\|_2$ can be solved in a numerically stable way using the QR-factorization of A . However, in several applications, e.g. when A is sparse, the orthogonal factor Q may not be available. Then the solution is generally computed from the "semi-normal equations" $R^T R x = A^T b$. It is easily shown that this method is not stable. We show that by a refinement step using only single precision the stability of the QR-method is almost recovered. Applications of this to the updating of a sparse R-factor of A , when appending a column is discussed.

A Fourier-Spectral-Method for the Stokes-Resolvent

W Borchers, University of Paderborn, Germany.

The numerical construction of the Stokes-Resolvent in a bounded threedimensional domain via Boundary Element Methods requires the solution of the corresponding inhomogenous problem with non-prescribed boundary values. The usual volume potential is replaced by a solenoidal trigonometric series (i.e. by the eigenfunction expansion of the Stokes-Resolvent in the case of periodic boundary conditions in a cube).

It is shown, that the rate of decay of the truncation error depends on the smoothness of the solution and is more than algebraic, whenever the solution is infinitely smooth. When the product trapezoidal rule is used, this result holds even then, when the discretization error is included.

On account of the incompressibility condition the boundary integral equation is not uniquely solvable. We split off the unknown eigenfunction with the help of the known adjoint eigenfunction, and we show, that the resulting integral equation is uniquely solvable.

Some Remarks on the Representations of Splines as Boolean Sums

L Bos*; P Lancaster; K Salkauskas, University of Calgary, Canada.

If P and Q are two projectors then under certain conditions, their Boolean sum, $P \oplus Q$, defined by $P \oplus Q = P + Q - PQ$ is well defined. If Q is a projection into a (relatively small) class of polynomials and P a more general interpolatory projector, then $P \oplus Q$ is an interpolatory projector which preserves this class of polynomials. A number of interpolation schemes such as kriging and thin plate splines naturally have the structure of a Boolean sum. We show that any interpolation which preserves polynomials of a certain degree can be expressed, at least formally, as a Boolean sum. Further we show that, in one variable, any spline interpolant not suffering a certain, slight defect can also be written as a particular Boolean sum. Some related questions are also discussed.

Constrained Optimization Using Piecewise Quadratic Functions

R Bramley, University of Cambridge and University of Illinois-Urbana, U.S.A.

An algorithm for solving inequality constrained minimization problems is presented. The algorithm is iterative, with an unconstrained minimization performed on a piecewise quadratic function on each iteration. By using an augmented Lagrangian line search function, global convergence properties are established. Also, the method is shown to be locally identical to the dual variable metric method of Han and hence has a superlinear convergence rate. Finally, preliminary computational results are presented.

Antisymmetric Matrices, Staircase Functions and LP

C G Broyden, University of Essex.

This paper outlines a proof of the Theorem that, for any real $A = -A^T$ there exists an $x \geq 0$ such that $Ax \geq 0$ and $x + Ax > 0$. It shows that, if $x(\theta)$ is such an x corresponding to the matrix $A + \theta(pq^T - qp^T)$, where θ is a scalar parameter, $p, q \in \mathbb{R}^n$, $p, q \geq 0$ and $p^T q = 0$ then if $r(\theta) = q^T x(\theta) / p^T x(\theta)$, $r(\theta)$ is a "staircase function" of θ and is multi-valued on a finite set of values of θ .

The use of these "staircase functions" not only facilitates the proof of the Theorem but enables several (somewhat inefficient at present) algorithms for solving the general LP problem to be constructed.

Finally, it is shown that Farkas's Theorem, and other duality theorems, are but special cases of the above Theorem.

Long Vectors for Quasi-Newton Updates

A Buckley, Dalhousie University, Canada.

This talk will demonstrate a technique for deriving standard weighted quasi-Newton update formulae. The method uses direct products and other very large matrices and vectors, some constructed specially for the symmetric case. The motivation for interest in these techniques is their applicability to special problems, including those with structure or those which are sparse.

Extended Backward Differentiation Formulae for Stiff Differential Systems

J R Cash, Imperial College.

Modified extended backward differentiation formulae have been shown to be very promising for the numerical integration of stiff systems of ordinary differential equations. In this talk we describe a number of ways in which their performance can be improved. In particular we examine efficient methods for solving linear differential systems, ways of improving the solution of the nonlinear algebraic equations and methods for solving inherently unstable problems.

Linear Stability of Diagonally Implicit General Linear Methods
 F Chipman*, K Burrage, *Acadia University, Canada.

We consider the general linear method

$$Y_i = \sum_{j=1}^r a_{ij}^{(1)} y_j^{(n-1)} + h \sum_{j=1}^s b_{ij}^{(1)} f(x_{n-1} + hc_j, Y_j) \quad i = 1, \dots, s$$

$$y_i^{(n)} = \sum_{j=1}^r a_{ij}^{(2)} y_j^{(n-1)} + h \sum_{j=1}^s b_{ij}^{(2)} f(x_{n-1} + hc_j, Y_j) \quad i = 1, \dots, r$$

for the solution on the initial value problem

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \quad f: \mathbb{R}^{m+1} \rightarrow \mathbb{R}^m.$$

The Y_i approximate the solution at the points $x_{n-1} + hc_i$ and are only used within a step. The $y_i^{(n)}$ carry information from step to step.⁽¹⁾ The method is diagonally implicit if the matrix $B_1 = (b_{ij}^{(1)}) = L + \lambda I$, where L is strictly lower triangular. We consider two cases in which

i) $y_i^{(n)} \approx y(x_{n-i})$, a multistep-type method and,

ii) $y_i^{(n)} \approx \frac{h^{i-1} y^{(i-1)}(x_n)}{(i-1)!}$, a Nordsieck-type method.

The linear stability of these families will be discussed and numerical evidence of higher order A-stable methods will be presented.

Application of Approximation Theory to the Solution of Singular Boundary Value Problems

L Collatz, University of Hamburg, W. Germany.

The lecture begins with a short historical survey with the progress of approximation theory from Weierstrass, Tschebyscheff a.o. over the generalizations by Haar to multivariate functions $u(x_1, \dots, x_n)$. One is approximating the wanted function u by functions w of a certain class W of functions depending on parameters. One can see with aid of the inclusion theorems of the approximation theory for the minimal distance, which degree of accuracy is possible using the class W . This is illustrated on different recently considered numerical examples of partial differential equations with singularities.

Numerical Results for a Novel Method for Solving an Inverse Problem
for Time Harmonic Acoustic Waves

D Colton and P Monk*, University of Delaware, U.S.A.

Using Herglotz wave functions, a novel method for determining the shape of an acoustically soft obstacle from a knowledge of the time harmonic incident wave and the far field pattern of the scattered wave will be presented. Theorems concerning the uniqueness and continuous dependence of shape of the obstacle on the data (assuming certain reasonable a priori information) will be discussed. Finally, numerical results showing the practicality of the method will be presented.

On numerical methods for continuous location problems, including
the handling of degeneracy

A R Conn, University of Waterloo, Canada.

Continuous location problems are potentially difficult to solve because the objective function is not every where differentiable. An algorithm based upon the solution of a finite sequence of linearly constrained subproblems is presented. Descent directions for these subproblems are obtained by projecting the Newton direction onto the corresponding constraint manifold. Univariate minimization is achieved via a specialised linesearch which recognises the possibility of first derivative discontinuity (and second derivative undoubtedness) at points along the descent direction.

The algorithm extends earlier results of the authors and relates to methods recently described by Overton and Dax. In particular, it is known that degeneracy complicates the numerical solution of location problems. This degeneracy is identified and a method that circumvents the degeneracy is included.

An implementation of the algorithm that exploits the intrinsic structure of the problem is described along with a discussion of numerical results.

Adaptive Self-Validating Numerical Quadrature

F Corliss, Marquette University, Milwaukee and MRC, University of Wisconsin, U.S.A.

SVALAQ (Self-Validating Adaptive Quadrature) is a suite of programs which use methods of interval mathematics to give guaranteed bounds for numerical quadrature. The set of all possible answers to the problem posed is validated to lie within the interval computed by SVALAQ. The integration uses Gaussian quadrature rules. Newton-Cotes closed formulas, and rules for Taylor polynomials. The interval value of the remainder term for the rule selected is generated by automatic differentiation. Both order adaptive strategies and subinterval adaptive strategies use guaranteed bounds for the integral on each subinterval. Certain types of singularities are recognised and handled. The integration terminates when the noise in function evaluation prevents further improvements in the accuracy of the integral. SVALAR can even validate that some integrals are undefined. Numerical examples are included.

On the numerical solution of 3 - dimensional linear elliptic partial differential equations

D S Daoud, Scientific Documentation Centre, Baghdad.

A linear elliptic partial differential equation defined in R^3 is approximated using finite difference approximation.

The generated matrix from this approximation is a 7-diagonals sparse matrix, a particular class of regular splittings of the generated matrix is proposed.

A comparison will take place to show the efficiency of such a matrix decomposition by solving several model problems iteratively.

Error Bounds for Implicit Runge-Kutta Methods in the Solution of Stiff Nonlinear Differential Equations

K Dekker, University of Leiden, The Netherlands.

We consider the class of ordinary differential equations

$$(1) \quad y'(x) = f(x, y(x)), \quad y(x_0) = y_0, \quad f: R^{n+1} \rightarrow R^n,$$

which satisfy the one-sided Lipschitz condition

$$\langle f(x, y) - f(x, z), y - z \rangle \leq \nu \|y - z\|^2, \quad \forall y, z \in R^n, \quad x \geq x_0.$$

We analyse the behaviour of implicit Runge-Kutta methods applied to this class of equations, and we derive local and global error bounds for the numerical solution of the form

$$C(\nu h) h^q M,$$

where h stands for the stepsize, and M is a bound for certain derivatives of the exact solution of (1).

Results on the order of B-convergence of several well-known classes of Runge-Kutta methods (Gauss, Radau I and II, Lobatto) will be given. We conclude with some numerical illustrations.

A Wronskian Approach to the Eigenvalue Problems of Linear Differential Operators

M Demiralp, Research Institute for Basic Sciences, Turkey.

In this work, a method without any integration is proposed to determine the discrete spectrum of a linear differential operator (H), bounded from below. Main idea of this method is based on the fact that the ratio $H\psi/\psi$, being an eigenfunction of H , does not change over the whole domain of independent coordinates appearing in the structure of H . Although this constancy of local expectation, $H\psi/\psi$, is destroyed when ψ is not a true eigenfunction, one can, however, utilize this ratio to determine approximate values of low lying eigenvalues. Indeed, if we take ψ as a finite linear combination of suitably chosen basis functions φ_j ($j=1, \dots, N$) we can equate the first N derivatives of $H\psi/\psi$ to zero for the determination of arbitrary linear combination coefficients. This, however, yields a matrix eigenvalue problem $Ax = \lambda Bx$ where B and A are respectively Wronskian matrices of φ_j 's and u_j 's ($u_j = H \varphi_j$) and x denotes N -dimensional linear combination coefficient vector.

In this work, beside the formulation of the method some criteria for the choice of φ_j 's are discussed and some convergence properties of the scheme are presented.

Finally, some illustrative applications complete this work.

A High Order Leap Frog Scheme for Hyperbolic Systems

D B Duncan, Atomic Energy of Canada Limited.

A leap frog scheme for the approximate solution of systems of linear, variable coefficient hyperbolic equations is presented. The scheme is accurate to fourth order in time and space and has the same stability properties as the standard second order leap frog scheme.

The new scheme is easy to implement for multi-space-dimensional problems and its execution cost is about three times that of the second order leap frog on the same mesh.

The application of the scheme is illustrated for wave propagation problems in one and two dimensions.

On Measures of Nonnormality of Matrices

L Elsner; M H C Paardekooper*, Tilburg, The Netherlands.

Several measures of nonnormality of matrices, i.e. nonnegative functions m such that $m(A)=0$ iff A is normal, have occurred in the literature. We introduce new ones and give in particular comparisons between them. Some of these comparisons manifest wellknown phenomena of illconditioned eigenproblems.

Some of the studied measures are

$$m_1(A) : = \min\{\|A-N\|_F \mid N \in \mathcal{N}\};$$

$$m_2(A) : = \|\Lambda\Lambda^* - A^*A\|_F;$$

$$m_3(A) : = (\|A\|_F^2 - \sum |\lambda_i|^2)^{\frac{1}{2}};$$

$$m_4(A) : = \|\Lambda\Lambda^* - (A^*A)^{\frac{1}{2}}\|_F;$$

$$m_5(A) : = \min\{\|U-V\|_F \mid UAV^* \in \mathcal{D}, U, V \in \mathcal{U}\};$$

$$m_6(A) : = \min\{\|U-V\|_F \mid U^*(A+A^*)U, V^*(A-A^*) \in \mathcal{D}, U, V \in \mathcal{U}\};$$

$$m_7(A) : = \min\{\|X\|_2 \|X^{-1}\|_2^{-1} \|X^{-1}AX - \text{diag}(\lambda_j)\|_2\};$$

$$m_8(A) : = \min\{(\sum |\lambda_j|^{-\alpha_{p(j)}} + i\beta_{q(j)})^2\}^{\frac{1}{2}} \mid p, q \text{ permute } \{1, \dots, n\}\},$$

where $\mathcal{N}$, $\mathcal{D}$, $\mathcal{U}$ are the sets of normal, diagonal, unitary matrices, $\{\lambda_j\}$, $\{\alpha_j\}$, $\{\beta_j\}$ the eigenvalues of A , $(A+A^*)/2$ and $(A-A^*)/2$ resp.

A Composite Hopscotch Method of Increased Accuracy

D J Evans; A Danaee*, *University of Isfahan, Iran.

The Hopscotch point and block methods are well-known as a fast P.D.E. solver. However due to the term involving $\Delta t^3/\Delta x^2$ in the local truncation error, the same as the Du-Fort Frankel, the methods suffer from an inconsistency phenomena which bounds the users to apply small time increment.

Recently, Evans and Danaee (1982) developed a new block Hopscotch algorithm which is shown to be more efficient for the solution of partial differential equations. In this paper, it is shown that by a judicious combination of both point and block hopscotch algorithms, a composite method of greater accuracy can be obtained, which also remedies the inconsistency phenomena in the method.

Methods of Computation of Critical Points of Nonlinear Functionals
 A Eydeland, University of Massachusetts at Amherst, U.S.A.

In this paper the method of transformation of the objective functional is presented as a general approach to a problem of finding critical points of nonlinear functionals. Particular attention is given to non-convex problems, constrained problems, and problems of the mountain pass lemma type. Specific applications are discussed including numerical solution of the minimal surface obstacle problem, computation of periodic solutions of non-linear Hamiltonian systems and solving semilinear boundary value problems. Different aspects of numerical implementation of the method of transformation of the objective functional, such as global convergence, mesh refinement for nonlinear problems, etc., are discussed.

On the Numerical Solution of Engineering Boundary Value Problems
 G Fairweather, University of Kentucky, U.S.A.

The modelling of many problems in engineering leads to two-point boundary value problems for ordinary differential equations (BVODEs). Traditionally these problems have been solved numerically using ad hoc simple shooting techniques, which have proved to be reasonably useful for the solution of simple problems, but, in general, they have many deficiencies. In recent years, several robust, general-purpose software packages for solving systems of nonlinear BVODEs have been developed, the use of which has lead to the solution of problems which are difficult to solve if not intractable using shooting methods. The purpose of this paper is to demonstrate the effectiveness of two such packages for the solution of several rather difficult BVODEs arising in mechanical engineering and chemical engineering.

The first package, COLSYS, Algorithm 569 of the ACM TOMS library, implements the method of spline collocation at Gaussian points, in which the desired solution is approximated by piecewise polynomials represented by terms of a B-spline basis. The second package, DVCPR, from the IMSL library, implements a variable-order finite difference method based on the trapezoidal rule with deferred corrections. This code is one of the most recent versions of PASVA3, a package developed by V. Pereyra and his co-workers. Other versions of PASVA3 appear in the Harwell Subroutine Library (DD04AD) and the NAG library (D02RAF).

In this paper, COLSYS and DVCPR are used to solve accurately, efficiently and reliably a variety of BVODEs from the chemical engineering and mechanical engineering literature. In several instances, the packages produce results quite different from those appearing in the literature, raising doubts about the validity of the published results.

Quintic Spline Interpolation

T Fawzy, Suez Canal University, Egypt .

A method for solving the problem of finite interpolation using quintic splines is presented. A special kind of g-spline is constructed. The existence and uniqueness of the spline interpolant are investigated. The method is completely local and error bounds satisfying the saturation theorem are obtained for functions $f \in C^3[0,1]$. The method defined here, in contrast to many other methods does not require any end conditions.

A New Approach to Quasi-Newton Methods

J A Ford; A F Saadallah, University of Essex.

The secant equation, which underlies all quasi-Newton methods, stems from the use of a linear function to model the gradient along a chosen search direction. This paper presents five new optimisation algorithms derived from replacing this linear model by a more general model with a free parameter which is determined by using information contained in the current approximate Hessian. Using such a model can also give more flexibility in the termination criteria to be satisfied during the line search routine. It is shown that these new techniques may be expected to degenerate to the standard quasi-Newton strategy as the minimum is approached. The results of numerical experiments show that some of the new methods yield a significant improvement (up to 10%) in performance, for little or no additional computational cost.

A Variant of Karmarkar's Linear Programming Algorithm for Problems in Standard Form

D M Gay, AT&T Bell Laboratories, U.S.A.

This talk presents a variant of Karmarkar's linear programming algorithm that works directly with problems expressed in standard form and requires no a priori knowledge of the optimal objective function value. Rather, it uses a variation on Todd's approach to compute ever better bounds on the optimal value, and it can be run as a primal-dual algorithm that produces sequences of primal and dual feasible solutions whose objective function values converge to this value. The only mildly restrictive assumption is that the feasible region is bounded with a nonempty interior.

Linear Multistep Methods for Functional Differential Equations

N de Gee, Agricultural University, The Netherlands.

Two different ways to define linear multistep methods for functional differential equations are described, and some of their properties are compared. The asymptotic behaviour of the global discretization error is investigated. Finally, Milne's device is generalized to FDEs. The effect of the non-smoothness of the exact solution is taken care of.

An Interior-Point Method for Linear Programming and its Equivalence to Karmarkar's First Projective Method

P E Gill; W Murray; M A Saunders; J A Tomlin; M H Wright*,
Stanford University, U.S.A.

We derive an interior-point method for linear programming by applying a logarithmic barrier transformation and performing Newton steps for a sequence of barrier parameters. This "Newton barrier method" can be interpreted as a parameterized version of Karmarkar's first (1984) projective method for linear programming, and is shown to be equivalent to that method under certain conditions. Numerical results for several test problems indicate the promise of the interior-point approach.

Differentiable penalty function methods for solving the nonlinear ℓ_1 problem

N I M Gould, University of Waterloo, Canada.

In this talk we shall describe new methods for minimizing the one-norm of a (nonlinear) vector valued function (the nonlinear ℓ_1 problem). The methods are all based upon the classical reformulation of the ℓ_1 problem as a nonlinearly constrained minimization problem. The resulting nonlinear program is solved using simple differentiable penalty function techniques. The interesting features are that (i) the ill-conditioning normally associated with such penalty functions is avoided and (ii) account is taken of the structure of the problem to produce special (aesthetically pleasing) penalty functions.

The relative distance of J.D. Pryce in ℓ_∞^n
W Govaerts, State University of Gent, Belgium.

Continuing work of F.W.J. Olver, J.D. Pryce ('A new measure of relative error for vectors', SIAM, J. Numer. Analysis 21 (1984) 202-215) define a new measure of relative error for vectors. If x, y are two nonzero vectors in a Banach space E (usually $\mathbb{R}^n$), then he defined

$$\rho(x, y) = \inf_C \left\{ \int_C \frac{\|dx\|}{\|x\|} : C \text{ is a smooth path from } x \text{ to } y \right\}.$$

With this definition, $E \setminus \{0\}$ becomes a metric space. Up to second order terms, $\rho(x, y)$ equals $\|x - y\| / \|x\|$ and good bounds are available. With respect to actual calculations, $\rho(x, y)$ behaves in a much nicer way than $\|x - y\| / \|x\|$ and so seems to be quite useful in error theory.

Until now, explicit formulae for $\rho(x, y)$ are known almost exclusively in the case of Hilbert space. This is undoubtedly the most important situation; nevertheless for a better understanding one would like to know what happens in other familiar spaces. We give a complete answer (including geodesic lines) in ℓ_∞^2 and a partial solution in ℓ_∞^3 ; in some cases the last results extend to ℓ_∞^n for any finite n .

Accurate Calculation of Linear Functionals of Solutions of certain Integral Equations

I G Graham, University of Bath.

Integral equations of the form

$$y(s) = f(s) + \int_0^1 k\left(\frac{s}{\sigma}\right) y(\sigma) \frac{d\sigma}{\sigma}, \quad s \in [0,1] \quad (1)$$

where y is to be found arise in a variety of contexts. Putting $s = e^{-t}$, $\sigma = e^{-\tau}$ converts (1) to the familiar Wiener-Hopf equation

$$y(e^{-t}) = f(e^{-t}) + \int_0^{\infty} k(e^{-(t-\tau)}) y(e^{-\tau}) d\tau,$$

which arises classically in the theory of radiative transfer. More recently (1) has arisen, for example, when particular boundary value problems in elasticity are solved using integral transforms and dual integral equations, and, more generally, in the theory of regularity of solutions to boundary value problems in domains with corners.

Here we discuss some properties of equation (1) and its numerical solution by Galerkin and certain collocation methods. In particular we show how to obtain high order accurate approximations to linear functionals on the solution y , and apply this to the calculation of stress intensity factors for a particular problem in elasticity.

On a Method for the Simultaneous Determination of the Zeros of a Polynomial

J A Grant, University of Bradford.

In a recent paper, Pasquini and Trigiante (Math. Comp. 44, 1985, pp.135-149) proposed a globally convergent method for simultaneously finding polynomial zeros. Instead of using a method based on the solution of Vieta's equations, they use a formulation involving divided differences. Here, some preliminary findings are reported on a comparison of this approach with the more usual formulation.

Equilibrium States of Runge Kutta Schemes

G Hall, University of Manchester.

Understanding the behaviour of Runge-Kutta codes when stability considerations restrict the stepsize provides useful information for stiffness detection and other implementation details. Analysis of equilibrium states on test problems is presented which provides predictions and insights into this behaviour. The implications for global error are also discussed.

Overlapping Runge-Kutta Methods

P J Harley; J D Lambert *; University of Sheffield, University of Dundee.

A class of Runge-Kutta methods which make maximum use of the stages from previous steps is derived, resulting in very economical implementation. The methods are essentially block methods, but the size of the block is unlimited; in practice the method starts a new block only when a step-change is required. A third order member of this family requires four evaluations for the initial step and only one evaluation at every subsequent step (of constant length), an error estimate being available at the cost of an optional additional evaluation. Step-changing can be achieved simply and reasonably economically. The methods are easy to program and are thought to be suitable for microcomputer use.

Efficient Boundary Element Methods for Three-Dimensional Viscous Flows

F K Hebeker, University of Paderborn, W. Germany.

Recently the numerical investigation of boundary element methods for viscous flow problems has been tackled by several authors. In this talk we plan to comment on the state-of-the-art of an efficient Stokes solver of boundary element type to solve the boundary value problems of 3-D viscous incompressible fluid flows in arbitrary (particularly unbounded) flow regions.

Roughly speaking, our Stokes solver consists of three components:

- . a spectral method to handle the nonhomogeneous part of the differential equations;
- . a boundary element method (heart of the matter) to adapt to the given boundary data;
- . a multigrid method to solve efficiently the resulting algebraic system.

This talk will include a short treatment of the mathematical foundations, a more detailed convergence analysis of the approximation procedures, and will be completed with 3-D numerical test computations.

Finally some recent applications to the full (nonstationary and nonlinear) Navier Stokes equations at moderate Reynolds number are discussed.

Recurrence in the Nonlinear Schrodinger Equation

B M Herbst*; J A C Weideman, University of the Orange Free State, Bloemfontein, South Africa.

The x-independent solution of the nonlinear Schrödinger equation

$$i u_t + u_{xx} + q|u|^2 u = 0$$

is given by $u = A e^{iq|A|^2 t}$. It is well-known that this solution is unstable to perturbations of sufficiently low frequency. The resulting unsteady solution is known to display recurrence. This behaviour will be investigated by means of Fourier methods. Theoretical and numerical results will be given.

The Numerical Stability of Two Matrix Newton Iterations
 N J Higham, University of Manchester.

We examine the behaviour in finite precision arithmetic of two Newton iterations, the first for computing the matrix square root and the second for computing the nearest orthogonal matrix. The two iterations are closely related and for suitable choice of starting matrices both iterations are quadratically convergent. However, by means of a perturbation analysis and supportive numerical examples it is shown that while the second iteration is well-behaved, numerically, the square root iteration suffers from numerical instability. The instability can be sufficient to cause the computed sequence of iterates to diverge, even though the corresponding exact sequence of iterates is mathematically convergent.

Improved Implementation of the Pivoting Strategy in Sparse Matrix Techniques

N Houbak, Technical University of Denmark.

Pivoting is used in Sparse Matrix Technique (SMT) mainly to reduce the number of fill-ins generated during the elimination and thereby reduce the overall costs (storage and computing time). The cost of the pivoting consists of two parts: 1) Search for the pivot element and 2) exchange the rows/columns (logical or physical). This lecture mainly concerns the second part.

Physical exchange of row and column numbers is a very expensive process in SMT, since it involves quite a lot of searching in the structure. Logical exchange of rows/columns requires additional storage for 2N INTEGERS, and worse of all, at the innermost loop one extra array addressing is needed. The lecture will show how this cost can be eliminated.

The second part of the lecture will concern the improvement of the iterative refinement technique used in connection with a drop tolerance.

Predictor-Corrector Methods for Periodic Second-Order Initial-Value Problems

P J van der Houwen*; B P Sommeijer, CWI Amsterdam, The Netherlands.

Recently, various papers have been published dealing with increasing the phase lag order of methods for the special second-order equation

$$(1) \quad y''(t) = f(t, y(t)).$$

Relative to a linear test equation, one may distinguish papers which deal with reducing the phase lag (or: phase error, dispersion) of the homogeneous solution component and papers which deal with reducing the phase lag of the inhomogeneous component.

In this lecture, we shall be concerned with methods that produce solutions with small phase lag in the homogeneous solution component. A particularly attractive method of this sort was proposed by Chawla and Rao. Their method is explicit, has algebraic order 4 and phase lag order 6. Moreover, since only 3 right-hand side evaluations per step are involved, the interval of periodicity, which is given by $[0, 7.56]$ (in the sense of Lambert and Watson) is relatively large.

Motivated by the result of Chawla and Rao we have looked for methods with both higher algebraic and phase lag order. As starting point we have chosen a generalization of predictor-corrector methods. Such methods have been analysed for first-order equations; a straightforward modification of these methods make them applicable to second-order equations of type (1). Within the class of these predictor-corrector methods we shall construct numerical schemes with algebraic order 4 and 6, and with phase lag orders up to 10. In fact, it is possible to obtain arbitrarily high phase lag orders by increasing the number of stages (corrections) in the numerical scheme. Similarly, by starting with a corrector of appropriate algebraic order we can obtain any algebraic order we want.

By numerical examples we show that these methods are considerably more accurate than conventional methods in linear and weakly nonlinear problems where the homogeneous solution components dominate.

A Study of B-convergence of Runge-Kutta Methods

W H Hundsdorfer*; K Burrage; J G Verwer: Centre for Mathematics and Computer Science, Amsterdam.

In this paper convergence results are presented for implicit Runge-Kutta methods applied to stiff semi-linear systems of differential equations

$$U'(t) = QU(t) + g(t, U(t)).$$

The convergence results are independent of the stiffness of the system (B-convergence [1]). The results show that for many methods the order of convergence is larger than the order of the local errors (the stage order), a phenomenon which has been often observed in numerical experiments ([1], [2]).

- [1] R. Frank, J. Schneid, C.W. Ueberhuber: Order results for implicit Runge-Kutta methods applied to stiff systems, Report 53/82, Techn. Univ. Vienna; to appear in SIAM J. Num. Anal.
- [2] K. Dekker, J.G. Verwer: Stability of Runge-Kutta methods for stiff nonlinear differential equations, North-Holland, Amsterdam 1984.

The Numerical Solution of Elliptic Free Boundary Problems using Multigrid Techniques

R Hunt, University of Strathclyde .

A multigrid algorithm is developed for the numerical solution of elliptic free boundary problems. The domain of the problem is mapped onto a rectangle and the governing equations discretised using finite differences. The resulting algebraic system is solved iteratively using a multigrid V cycle. For a convergent relaxation procedure it is necessary to use line iteration perpendicular to the free boundary simultaneously altering the values of the dependent variable and the position of the boundary, which is conveniently done using a single Newton iterate. Three problems are considered, a Poisson type problem, a steady state heat transfer problem and one from electrochemical machining. The first two problems rapidly converged in a few multigrid cycles, the third converged less rapidly though adequately. Since full multigriding (FMG) is used, the results on the three finest grids could be combined to give accurate results of sixth order.

Boundedness of Solutions of Difference Equations and Application to Numerical Solution of Integral Equations

Z Jackiewicz, University of Arkansas, U.S.A.

We study the boundedness of solutions of the difference equation of the form

$$\sum_{i=0}^r (\alpha_i + n^{-1} \beta_i) y_{n-i} = 0$$

$n = r, r+1, \dots$, which is a special case of difference equations of Poincare type.

The following result has been established: Assume that the polynomials

$$\phi(\xi) = \sum_{i=0}^r \alpha_i \xi^{r-i} \quad \psi(\xi) = \sum_{i=0}^r \beta_i \xi^{r-i},$$

have no common factor and that ϕ is a simple von Neuman polynomial with essential roots $\xi_1, \xi_2, \dots, \xi_k$. Then every solution of (E) is bounded provided that

$$\frac{1}{2} \pi \leq |\text{Arg}(\xi_i) - \text{Arg}(\gamma_i)| \leq \frac{3}{2} \pi$$

where $\gamma_i = -\psi(\xi_i)/\phi'(\xi_i)$, $i = 1, 2, \dots, k$.

This result is useful in stability analysis of some numerical methods for Volterra integral equations of the first and second kind and Volterra integro-differential equations. (These results were obtained jointly with V.L. Bakke.)

Accuracy barriers of full discretizations of $u_t = u_x$
 R Jeltsch*; J H Smit, RWTH Aachen, Germany.

The full discretizations

$$s(\mu, E) U(x, t + \Delta t) = r(\mu, E) U(x, t)$$

is considered. Here the operator E represents a shift by Δx in space direction, μ is the Courant number $\mu = \Delta t / \Delta x$ and $z^R s(\mu, z)$, $z^r r(\mu, z)$ are polynomials in z of degree $R+S$ and $r+s$, respectively. $s(\mu, z)$ is assumed to be normalized such that $s(\mu, 1) = 1$. Further it is assumed that $s(\mu, z) \neq 0$ for $|z| = 1$ and that R is the number of zeros of $s(\mu, z)$ in $|z| < 1$. Then it is shown for all Courant numbers $\mu \in (0, 1)$ that the order of accuracy p of a stable scheme is bounded by $q := \min \{2s + 2S, 2r + 2R + 2\}$. In addition if $p = q$ then we can give an explicit bound for the best possible error constant. The proofs are done by comparing the general scheme to certain F  d   schemes using order stars.

Moving Finite Elements for Nonlinear Diffusion Problems
 I W Johnson, University of Reading.

The Moving Finite Element (MFE) method is applied to nonlinear diffusion equations of the form $u_t = [u^n u_x]_x$ [$n > 0$], whose solutions exhibit steep moving fronts. After an appropriate change of dependent variable we derive semi-discrete MFE equations which give the position of the moving interface exactly and also derive a maximum principle for the gradient of the MFE approximation. No regularization terms are needed and explicit time stepping is found to be sufficient to obtain a good solution in time.

Numerical results in one dimension are compared with similarity solutions. Extension and implementation of the method to similar problems in two space dimensions is also discussed.

Integration Formulae for Singular Functions over the Triangle.
 P. Keast*; M. Hollosi, Dalhousie University, Canada.

Boundary element methods for three dimensional partial differential equations lead to linear or algebraic equations for the coefficients of the basis functions. These equations involve integrals over surface elements, usually triangles, of functions having singularities of known type at the corners of the triangles. Classical polynomial based integration formulas do not perform very well on such integrands, and can be expensive. Adaptive methods, designed to integrate non-smooth functions in a wide class, are effective on this type of function, but are inefficient largely because they do not take advantage of the fact that the nature and position of the singularities are known beforehand.

Given the form of the singularity, and its position, a more efficient approach is to use extrapolation on the asymptotic error series, eliminating the rational powers of the mesh size in turn. The asymptotic expansions were derived by Lyness and Monegato, (Maths. Comp. 1980), and Richardson extrapolation can be used. The resulting non-adaptive formulae promise to be as successful as, but cheaper than, adaptive polynomial based methods.

Numerical Behaviour of Cubic Quartic Spline Fits
 Ha-Jine Kimn, INRIA and Ajou University, Korea.

The theories and numerical methods to construct a spline fit from the data given as horizontal segments, rectangles of uncertainty, and combinations of them with vertical segments, are not well known. We have studied a numerical treatment to construct a spline fit from experimental data which are erroneous in two dimensional cartesian coordinate. Using the spline function theory for fitting (smoothing), we have introduced a representation of error on the data in abscissa and ordinate, and found a sufficiently regular function (cubic-quartic spline) $\sigma(t) \in H^2[a, b]$ such that

$$\int_a^b (\sigma''(t))^2 dt + \rho \sum_{i=1}^n \frac{1}{\epsilon_i^2} \left(\frac{1}{b_i - a_i} \int_{a_i}^{b_i} \sigma(t) dt - z_i \right)^2$$

$$= \min_{x \in H^2[a, b]} \left[\int_a^b (x''(t))^2 dt + \rho \sum_{i=1}^n \frac{1}{\epsilon_i^2} \left(\frac{1}{b_i - a_i} \int_{a_i}^{b_i} x(t) dt - z_i \right)^2 \right]$$

with $a \leq a_1 \leq b_1 < a_2 \leq b_2 < \dots < a_n \leq b_n \leq b$, $\epsilon_i > 0$, $\rho > 0$, and $z_i = x(t_i)$.

We have deliberated the second term of above expression which figures at the same time the error in abscissa represented by

$$\int_{a_i}^{b_i} x(t) dt / (b_i - a_i)$$

where a_i and b_i are the error bounds of the measurement in abscissa $t_i \in [a_i, b_i] = [t_i - \eta_i, t_i + \eta_i]$ with maximum deviation η_i around t_i and the error in ordinate represented by $1/\epsilon_i^2$ with the maximum deviation ϵ_i around z_i .

We have studied on the numerical technique to calculate above $\sigma(t)$ practically. With a kind of numerical results, we have remarked the influences by the change of data and coefficient $\rho > 0$. Some of these remarks can be explained theoretically and even numerically. At first when $\epsilon_i = 0$, all curves of each $\rho > 0$ pass always the same points. Moreover, if $\eta_i = 0$, the curve pass through the points (t_i, z_i) . If $\eta_i \neq 0$, the curve pass through the neighborhood of the points (t_i, z_i) . On the other hand, when $\epsilon_i \neq 0$, we get the empirical results. That is, the ϵ_i have much more influential than η_i and the curve concerned with the greatest coefficient $\rho > 0$ pass through the nearest point from the point (t_i, z_i) . Therefore our problem is nicely solved.

Multivariate Trigonometric B-splines

P E Koch, University of Trondheim.

A relation between univariate trigonometric and polynomial B-splines is extended to higher dimensions and used to construct a class of multivariate trigonometric B-splines from the multivariate polynomial ones. These new functions are trigonometric splines in each variable, but they are not tensor product splines. They are smooth and have local non-polygonal support. They possess a recurrence relation similar to that of the multivariate polynomial B-splines.

Formula Manipulation in Numerical Analysis

N Kückler, Universität GHS Paderborn, Germany.

A short hint shall be given about the possibilities of using formula manipulation with numerical problems.

First the abilities of the used system MAPLE shall become evident by some examples.

Then the application of MAPLE to numerical problems is discussed in general.

Finally the use of MAPLE in connection with a FEM - problem is demonstrated. An example is given with quadratic or cubic shape functions on two-dimensional triangular elements. One application with further investigations is the evaluation of the torsional rigidity of a prismatic section.

Parameter Selection Methods in the Regularisation of Ill-conditioned Linear Equations

A J MacLeod, Scottish College of Textiles.

Let A be a symmetric positive-definite matrix with

$$A \underline{f} = \underline{g}$$

and A very ill-conditioned.

Assume we don't know $\underline{g}$ but $\underline{g} + \underline{e}$, with only partial knowledge of $\underline{e}$.

$A^{-1}(\underline{g} + \underline{e})$ can be a very poor approximation to $\underline{f}$, so we consider approximations of the form

$$\underline{f}_\alpha = (A + \alpha I)^{-1} (\underline{g} + \underline{e}).$$

We look at five methods which have been proposed to select a good value of α :

- a) Residual method
- b) Quasi-solutions method
- c) Quasi-optimal method
- d) Ratio criterion method
- e) Generalised cross-validation method.

Theoretical and practical results are given to compare the effectiveness of these methods.

Parallel Algorithms for Time Dependent P.D.E's
I Martindale*; R Wait, University of Liverpool.

The N.A.G.F.E. Library (1) consists of FORTRAN subroutines, used in the numerical solution of partial differential equations employing the Finite Element Method.

The three major areas of application are:

- (i) Steady state problems.
- (ii) Time dependent problems.
- (iii) Eigenvalue problems.

In Wait and Martindale (2), details were given of parallel algorithms for two dimensional elliptic equations, with results obtained on the I.C.L.D.A.P., an "array processor", from software written in the highly parallel language D.A.P. FORTRAN.

We are currently interested in parallel algorithms for time dependent problems.

We have considered the diffusion and advection equations in one, and two, dimensions. A new block mass lumping scheme will be presented.

Regarding eigenvalue problems, we show how the inverse iteration algorithm can be "parallelised".

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A variable elimination algorithm for ℓ_1 quadratic programming
S P J Matthews*; R Fletcher, University of Dundee.

A promising approach to solving non-linear programming problems has been the use of successive quadratic programming problems to approximate the original problem. However this approach does have some difficulties of feasibility and boundedness which can be avoided by using successive ℓ_1 -quadratic programming subproblems.

In this paper we present an algorithm designed to solve such problems using an active set method and LU factors to represent constraint information. A variable elimination approach is used when constructing reduced problems. It is shown that great savings can be made by exploiting bounds intrinsic to the subproblem. A method for resolving degeneracy is presented that is also applicable to most other active set algorithms including the Simplex method for linear programming. Numerical comparisons are made with other recent algorithms.

Multistep Multiderivative Methods for Volterra Integro-Differential Equations

M Meneghette, Oxford University.

The ideas and theory of multistep multiderivative methods for solving ordinary differential equations are extended to Volterra integro-differential equations. A concept of zero-stability is given which, together with consistency, permits the derivation of an order of convergence result. It is noted that lower order quadrature formulae may be used in the evaluation of the integrals involved in the derivatives of the function F without any deterioration in the global order of convergence. Numerical results are presented using methods which are stiffly stable in the ordinary differential equation sense.

Defect Correction from a Galerkin Viewpoint

G Moore, Brunel University.

We consider the numerical solution of systems of nonlinear two-point boundary value problems by Galerkin's method. An initial solution is computed with piecewise-linear approximating function, which is then improved by using piecewise polynomials to compute defect corrections. This technique, including numerical quadrature, is justified by typical Galerkin arguments rather than the traditional asymptotic error expansions of finite difference methods, and we compare the final equations derived from each approach.

Type-Insensitivity for Stiff Codes

S P Nørsett, University of Trondheim, Norway.

In order to solve stiff systems effectively one is normally forced to use implicit methods. On the other hand the system might shift from stiff to non-stiff during parts of the integration interval. It is therefore of interest to construct the codes so that the automatically observe this change and can take the proper action. We discuss how to handle this problem by changing from Modified Newton iteration to fixpoint iteration and of course the opposite case is also handled. The key is to define the stiffness as the ratio between the residual norm and the displacement norm.

A "Repair" Algorithm for Constructing Non-Negative Splines

G Opfer, University of Hamburg, Germany.

In many situations non-negative approximations for positive functions are required. Typical examples of such positive functions are density functions occurring in probability theory. The proposed algorithm starts with the interpolating natural spline s as an approximation to a given positive function. Simple examples show that this spline may be in general negative between certain knots. Assume that I is an interval between two consecutive knots and that s is negative somewhere in I . Now a repair is executed by placing some additional knots in I and computing a non-negative approximation in I to $\text{Res } s/I$ which fits the spline s smoothly at the end of I . It is shown that such a construction is possible and how it behaves numerically. Joint work with M.L. Puri, Indiana University and P. Fischer, University of Hamburg is acknowledged.

Step Change Strategies for ODE Solvers
 O Østerby, Aarhus University, Denmark.

When solving systems of ordinary differential equations effectively it is necessary to be able to change the step-size during the course of integration. The commonly used techniques for computing a new step-size in connection with multistep methods are based on formulas derived in the fixed step-size case and are therefore not correct. The tendency is that by step-size increase the step is increased by too small an amount and by step-size reduction the step is not reduced enough. This latter effect is usually remedied by the incorporation of "safety-factors" (which serve other purposes, too) so existing codes seem to work quite well despite the wrong formulas.

In the paper we propose a set of correct formulas for step change in connection with Adams methods and demonstrate the effects on a set of test problems.

On the Numerical Stability of the Bartels-Golub and Fletcher-Matthews Algorithms for Updating Matrix Factorizations
 M J D Powell, University of Cambridge.

Several numerical procedures require the $n \times n$ system of equations $A_{k-k} x_k = b_k$ to be solved for $k = 1, 2, 3, \dots$, where, for each k , the matrix A_{k+1} is formed by changing just one column of A_k . In this case the work per iteration can be reduced from $O(n^3)$ to $O(n^2)$ by calculating a factorization of A_{k+1} from a factorization of A_k , but it can be difficult to achieve stability because few pivoting options are available. However, the Bartels-Golub and Fletcher-Matthews updating algorithms are usually highly successful, and moderate bounds have been found on the errors of each updating calculation. These two algorithms are described briefly, and it is noted that the Fletcher-Matthews method avoids an increase in the complexity of the factors as k increases, at the expense of higher error bounds.

The main purpose of this paper is to consider the worst errors that can arise from a sequence of updating calculations. A pathological example shows that when $n = 20$ the Fletcher-Matthews algorithm can lose 60 decimal places of accuracy, while the corresponding figure for Bartels-Golub is about 12 decimal places. We give some numerical results of computer calculations that correspond to pathological cases. A remedy is to re-factorize ab initio if a test indicates that unacceptable error growth may have occurred, but we find that a suitable test is not easily available for the Bartels-Golub algorithm. Therefore the obvious alternative of using iterative refinement when solving $A_k x_k = b_k$ may be preferable. Experience suggests, however, that both algorithms give good accuracy in practice.

Error Control of Prüfer Methods for Sturm-Liouville problems

J D Pryce, University of Bristol.

Automatic software is available for solving regular or singular Sturm-Liouville problems

$$(p(x)y') + (\lambda w(x) - q(x))y = 0, \quad a < x < b \quad (1)$$

with suitable BCs at a and b . One successful numerical method is a Prüfer transformation (to scaled polar coordinates r, θ in the py', y plane) followed by shooting. The problem then has the form: find λ such that there is a solution to

$$\theta' = F(x, \theta; \lambda), \quad \theta(a) \quad \text{and} \quad \theta(b) \quad \text{given.} \quad (2)$$

We study error control by regarding the numerical solution as computing $\bar{\lambda}$, the solution to a perturbed DE $\theta' = F(x, \theta; \lambda) + e(x)$ where $e(x)$ is a linear combination of δ -functions $e(x) = \sum e_i \delta(x - x_i)$ and e_i , the local errors at the integration meshpoints x_i , are approximated by an ODE-code's local-error estimates $\tilde{e}_i$.

Standard ODE theory gives expressions $\bar{\lambda} - \lambda = \sum J_i e_i$ where $J_i > 0$ come from the equation of first variation for (2). A special feature of Prüfer-based methods is that approximations $\tilde{J}_i$ to J_i come almost for free, leading to computable formulae

$$\bar{\lambda} - \lambda \approx \text{errest} = \sum \tilde{J}_i \tilde{e}_i,$$

$$|\bar{\lambda} - \lambda| \lesssim \text{errbnd} = \sum \tilde{J}_i |\tilde{e}_i|.$$

We argue: (1) some software is implicitly based on *errest*; while (2) error control using *errbnd* is more robust and (3) often remains robust in cases of pathologically close eigenvalues (eg quantum tunnelling problems) which cause severe difficulties to current codes.

On Finding the Minimum Norm on a Polytope

A Salamanca Fernández*; F J Prieto Fernández, ETS Ingenieros Industriales de Madrid, Spain.

Problems of calculating the minimum norm on a polytope often arise in algorithms related to non-smooth optimization. Although there exist finite methods for solving such a problem, their behaviour is unsatisfactory as the number of vertices grow. Three new approaches are described. Two of them are drawn from general nonlinear programming and the other comes from linear programming.

First, an adaptation of Newton method for nonlinear programming is discussed. The procedure requires various Newton steps due to the constraints in the problem. This is a finite algorithm which leads to the point of minimum norm, having the advantage of dealing with additional linear constraints on a numerical straightforward way.

Second, a normalized version of the reduced gradient method is proposed. Although this is not a finite process, its convergence has shown to be very fast, requiring a much lesser amount of computation effort per iteration than the previous method.

Finally an special version of Karmarkar techniques for linear programming has been developed. The method is again an infinite one, giving a good approximation to the solution if stopped at the first iterations. As in most cases an exact solution is not required - and even a rough approximation would be sufficient - this method proves extremely fast for very high dimension problems.

A New Analysis of Cosine Schemes for Second - Order Evolution Equations

S M Serbin, University of Tennessee, U.S.A.

We briefly recall a class of two-step schemes, known as "cosine methods" for second-order evolution equations. In lieu of previous analysis, which was based upon solution of second-order difference equations, we develop both the exact solution and the approximating scheme in terms of application of certain Chebyshev polynomial operators applied to the initial data. This formulation allows a streamlined stability and convergence analysis. Also, in analogy to a procedure for first-order evolution equations suggested by Baker and Bramble, we suggest a post-processing procedure for these cosine schemes, which allows one to employ a low-order approximation scheme up to the final time, then economically correct the approximation to obtain one of higher order.

Stability properties of linear multirate formulas

S Skelboe, University of Copenhagen, Denmark .

Consider a system of ordinary differential equations partitioned into a rapidly and a slowly varying sub-system:

$$\underline{y}' = \underline{f}(t, \underline{y}, \underline{z}) - \text{fast}$$

$$\underline{z}' = \underline{g}(t, \underline{y}, \underline{z}) - \text{slow}$$

Multirate methods exploit such a partitioning by integrating the slow sub-system with a larger steplength than the fast sub-system. Traditional integration methods use the steplength of the fast sub-system for the total system.

The present talk considers multirate formulas based on linear multistep formulas and interpolation formulas of Newton type. The slowly varying solution $\underline{z}(t)$ must be interpolated for the integration of the fast sub-system, and it is demonstrated how this interpolation is the main source of instability when integrating stiff systems of ordinary differential equations.

Multirate integration formulas can be organized according to various strategies. In the fastest first algorithm, the fast sub-system is integrated while the slow solution $\underline{z}(t)$ is extrapolated. In the slowest first algorithm, the slow sub-system is integrated a full step based on an extrapolated value of $\underline{y}(t)$. The slow solution $\underline{z}(t)$ is then interpolated during the solution of the fast sub-system.

The slow sub-system is usually integrated with a steplength being an integer multiple of the steplength for the fast sub-system. This implies that the fast sub-system is integrated at the same time instants as the slow sub-system, and these joint steps can be performed either semi-implicitly, i.e. implicitly in each sub-system, or fully implicitly for the total system.

These two pairs of algorithms lead to a total of four different organizations, all of which have been analyzed for stability properties. It is concluded that the fastest first algorithm with implicit joint step will have superior stability properties in general.

Since the interpolation/extrapolation of the slow solution is the main source of instability, it is natural to look for alternatives, and one such alternative, which has been analysed, is linear prediction. The slow solution $z(t)$ is assumed generated by a linear system which is identified. This system is then used for extrapolating $z(t)$. The preliminary results of this approach look promising, but with extrapolation of $z(t)$ based on linear prediction, the multirate formula is now nonlinear and as such much harder to analyse.

On Non-Linear Instability in Leap-frog Finite Difference Schemes
D M Sloan, University of Strathclyde.

Briggs, Newell and Sarie (1983) have discussed a mechanism for the destabilisation of finite difference approximations to nonlinear partial differential equations. Their ideas were developed using the leap-frog approximation to the advection equation. Here the same situation is examined in a manner which compares the basic solution to a periodic wavetrain. An investigation is made into the stability of the basic solution to small disturbances which take the form of side-band Fourier modes. The relation between side-band growth and envelope modulation is discussed.

W.L. Briggs, A.C. Newell and T. Sarie, J. Comput. Phys. 51, (1983), 83-106.

Time Dependent Hyperbolic Differential Equations and Variational Principles: Numerical experiments

I M Snyman, University of Dundee and Pretoria.

Suppose that you are given a one space dimension wave equation together with initial boundary conditions. Attempts to solve this well-known problem with the aid of variational principles will be discussed. The approach being followed does not depend on the linear properties of the initial value problem.

Tolerance Intervals in Numerical Solutions of First Order Ordinary Differential Equations

J R Ursell, Queen's University, Canada.

Consider the numerical solution of $\frac{dy}{dx} = f(x,y)$ with $y(x_0) = y_0$. Let $f(x_0, y_0) > 0$. Then, having chosen a step size h , consider $f(x,y)$ in the domain D given by $x_0 \leq x \leq (x_0 + h)$, $y_0 \leq y \leq (y_0 + k)$, where k is an estimated upper bound on the variation of y . Take a sample of n values of the random variable F in the domain D , where the value of F at (x,y) is $f(x,y)$. Let the lowest value in the sample be L , the highest V . If $hV < k$, we may reduce k to form a smaller domain D and repeat the procedure. If $hV > k$, reduce h and try again in the new domain D . Thus, we obtain a domain D and order statistics L and V . Let $p(f)$ be the probability distribution of F . It is known that if

$$\text{Prob} \left\{ \int_L^V p(f) df \geq q \right\} = \beta \quad (1)$$

where q and β are preassigned constants between 0 and 1 inclusive, then the LHS of (1) has for any order statistics L and V a value which does not depend on the probability distribution $p(f)$. The sample size n will depend to some extent on q and also on the required degree of certainty in the numerical solution, which depends on β . In general, we choose n to achieve the required β in (1) so that the LHS $\geq$ RHS. Then we can argue that if $y_1 = y(x_0 + h)$ for the actual solution of the initial value problem, then in D

$$\text{Prob} \left(L \leq \frac{y_1 - y_0}{h} \leq V \right) \approx \text{Prob} (L \leq f(x,y) \leq V)$$

The RHS has probability β of exceeding q . Hence we obtain a tolerance interval for y_1 .

The cases of $f(x_0, y_0) = 0$ and $f(x_0, y_0) < 0$ are similar. The method extends to several steps.

Runge Kutta Methods for ODE-problems with Discontinuities

P G Thomsen, Technical University of Denmark.

Initial value problems with discontinuities can be defined in the form

$$y' = \begin{cases} f_1(t,y) & \text{for } g(t,y) > 0 \\ f_2(t,y) & \text{for } g(t,y) < 0 \end{cases}$$

Where the switching function $g(t,y)$ is a given smooth function of t and y . In the neighbourhood of a discontinuity the problem may be treated as that of finding a zero of the function $g(t,y)$. For that purpose special interpolation formula derived from well known Runge Kutta methods are useful. An iterative scheme has been developed, the convergence properties of the iterative process will be presented. Numerical experiments have confirmed the efficiency of the process.

Attainable Eigenvalue Bounds for the Galerkin Mass Matrix
A J Wathen, University of Bristol.

In time-dependent finite element calculations, a mass matrix naturally arises. To avoid the solution of the corresponding system of algebraic equations at each time step, 'mass lumping' is widely used, even though this pragmatic diagonalisation of the mass matrix reduces accuracy.

We shall show how the unassembled form of finite element equations can be used to establish (in an element-by-element manner) attainable upper and lower bounds on the eigenvalues of the fully consistent mass matrix when pre-conditioned by its lumped form. We will give specific results for a number of different types of finite elements in 1,2 and 3 dimensions. The bounds are simply numerical values and are independent of the number of unknowns, and, for certain element types, even independent of the mesh irregularity. These results indicate that conjugate gradient methods are appropriate and very rapid for the solution of the algebraic equation system.

The ℓ_1 Solution of an Overdetermined System of Complex Linear Equations
G A Watson, University of Dundee.

A two-phase method is proposed for the ℓ_1 solution of an overdetermined complex linear system. The first phase is the solution of a certain real linear ℓ_1 problem, and the second consists of the application of Newton's method to an appropriate form of the characterization conditions.

Appropriate Inequality Constraints for Contact Problems of Elastic Beams and Plates

D R Westbrook, University of Calgary, Canada.

In dealing with contact problems of elastic beams and plates using finite element methods and a variational inequality formulation with the constraint that the solution be non-negative, a choice of constraints for the finite dimensional problem must be made. The obvious constraint, that nodal values of the solution be non negative, leads to satisfactory approximate values of the solution but does not always allow a simple estimation of the contact region to be made.

In the one dimensional case, with piecewise hermite cubics forming the finite dimensional space, inequalities of the form $u + \alpha hu' \geq 0$, $u - \alpha hu' \geq 0$ at each node, with h the element length and α a suitably chosen parameter, lead to simple estimation of the contact region with improved accuracy of solution at the nodes.

Unfortunately such inequalities do not seem to be easily generalized to higher dimensions.

Recently I have started to examine other linear inequalities of an element nature. In one dimension for example these take the form $u_0 + u_1 + \alpha h(u'_0 - u'_1) \geq 0$ where 0, 1 are the nodes of the element, h is the element length and α is a parameter ($\alpha = \frac{1}{4}$ implies that $u \geq 0$ at the mid point, $\alpha = \frac{1}{6}$ that $\int_e u dx \geq 0$).

The resulting quadratic programming problem has more complicated constraints than is usual and a penalty function approach was used to reduce all constraints to the form $v_i \geq 0$ for some vector of components v_i . In general this was not effective in defining the contact region but there were two exceptional choices of α which lead to great improvement. An examination of these cases is given.

Further work on the possibility of applying the method to the two dimensional case is currently underway.

Hybrid Method for Generalized Nonlinear Least Squares

Xu Chengxian, University of Dundee.

Hybrid method for nonlinear least squares is generalized to the solution of generalized nonlinear least squares problems, where the model may be nonlinear in its parameters and in the independent variables and all variables are subject to errors and the weights of all the readings are known. Experiments are described for comparing the results of the method with those of other existing techniques.

Efficient estimation of sparse Jacobian matrices by differences

T J Ypma, University of the Witwatersrand, South Africa.

In difference Newton-like methods for solving $F(x) = 0$, the Jacobian matrix $F'(x)$ is approximated by differences between values of F . If $F'(x)$ is sparse a consistent partition of the columns of $F'(x)$ can be exploited to approximate $F'(x)$ using relatively few values of F . We propose a general form for the differences involved, and provide a local convergence theory for the resulting methods. A superlinearly convergent stable cyclic secant method, in which at each iteration two values of F are required and several columns of the Jacobian matrix approximation are updated simultaneously, is developed.

Computational Results with A Trust Region Algorithm for Equality Constrained Optimization

Y Yuan, University of Cambridge.

A trust region algorithm for equality constrained optimization is given. At each iteration, a penalty function is introduced to calculate a trial step. Then another penalty function is used to test whether the trial step should be accepted. Computational results with the algorithm are discussed.

Variable stepsize variable formula method based on predictor-corrector schemes

Z Zlatev, Risø National Laboratory, Denmark .

The use of fairly general predictor-corrector (PC) schemes of linear multistep (LM) formulae in the numerical solution of systems of ordinary differential equations (ODE's) is considered. It is assumed that both the stepsize and the PC scheme can be varied during the computational process. The numerical methods obtained under these two assumptions are called predictor-corrector linear multistep variable stepsize variable formula methods (PC LM VSVFM's). The consistency, zero-stability and convergence properties of the PC LM VSVFM's are studied. Several results concerning these fundamental properties of the numerical methods are established. It should be emphasized that all theorems are formulated and proved under very mild assumptions on the stepsize selection strategy. The extension of the results for the so-called one-leg methods is briefly discussed. The use of PC LM VSVFM's leads to a very efficient treatment of many mathematical models describing different phenomena in science and engineering. Such methods have successfully been used in the numerical solution of systems of ODE's arising after the space discretization of some air pollution models.