

DUNDEE BIENNIAL CONFERENCE ON NUMERICAL ANALYSIS

UNIVERSITY OF DUNDEE

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ABSTRACTS

<u>Section A</u>	Invited talks
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<u>Section B</u>	Submitted talks
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SECTION A

Splines in Interactive Computer Graphics

Richard H Bartels, University of Waterloo, Canada

Computer graphics, particularly interactive computer graphics, is a relatively new field. It is not, as the name might imply, concerned with drawing graphs, but rather with the broadest issues of manipulating, transforming, and displaying information in visual format. It is interactive in so far as operations can be carried out in real time - which requires algorithms of high computational efficiency and low complexity.

The computer graphics community regards splines as a valuable tool, but it often applies them in a way not used by the mathematician. This difference raises computational issues which the numerical analyst might otherwise never see. This talk will provide a brief introduction to such issues and follow with a study of two current developments.

We begin with a review of the graphics environment, mentioning the modelling and display process and pointing out some of the costly issues. The major use of splines in interactive graphics comes through the construction of surfaces as averages of selected points in which B-splines are used as the weighing functions. Some examples will illustrate the characteristics of this style of "approximation".

With this material as background, we consider two recent developments. The first is the subdivision recurrence of Riesenfeld, Cohen, and Lyche, which will be given in its major details. The second is offered by Barsky's observations on geometric vs. mathematical continuity, and his introduction of Beta-splines, which will be described. Current research is concerned with a synthesis of these two developments. It would be desirable to generalize the Beta-spline and/or provide some sort of subdivision recurrence for it. We will close with some results (or possibly with some still open questions).

Some Methods for Separating Stiff Components in Initial Value Problems

Ake Bjorck, Linköping University, Sweden

When solving a stiff differential system by an implicit method, factorizing the Jacobian and solving the resulting linear equations often dominate the cost. We develop some methods related to a block Schur factorization of the Jacobian for separating the stiff components. These methods use a block version of the QR algorithm or, equivalently, a modification of simultaneous iteration. A few iterations are usually sufficient even when the separation between stiff and nonstiff eigenvalues is small. The methods are practical only for systems with relatively few stiff components.

Approximation order from smooth bivariate pp functions

Carl De Boor, University of Wisconsin-Madison, USA

The question of how smoothness requirements affect the approximation power of multivariate piecewise polynomial (=: pp) functions has been explored by R DeVore, K Hollig and the speaker, mainly in the simple context of

bivariate functions on a two-and three-direction mesh. A quick survey of these results is given, with special emphasis on the unresolved question: What is the precise relationship between approximation power and the existence of a suitable local partition of unity in the approximating pp space?

The Numerical Solution of Integral Equations with Weakly Singular Kernels
H Brunner, University of Fribourg, Switzerland

Integral equations of the second kind with weakly singular kernels possess solutions which, in general, have unbounded derivatives at one endpoint (Volterra equations) or at both endpoints (Fredholm equations) of the interval of integration. The presence of these singularities implies that numerical methods which exhibit a high order of convergence for equations with smooth solutions will now converge extremely slowly.

This talk will survey the use of collocation methods for the approximate solution of integral equations with weakly singular kernels. Even though our discussion will focus on integral (and integro-differential) equations of Volterra type, we shall also review recent results on the application of collocation methods to equations of Fredholm type, in order to reveal both similarities and contrasting features of collocation methods for these two classes of integral equations. In addition, numerical applications and open problems will be mentioned.

An Analysis of a Moving Finite Element Method for Convection-Diffusion Problems on Polygonal Domains

Todd F Dupont, University of Chicago, USA

A version of the Moving Finite Element Method of Keith and Robert Miller is treated. In this method the mesh for the finite element method evolves in time in accordance with a variational principle chosen to attempt to minimize the error. The evolution of the mesh can be viewed as a transformation of the domain on which the problem is posed. Conditions which guarantee that the resulting mesh is well behaved are presented and asymptotic error bounds are given. The question of error control is also discussed.

A Trust-Region Approach to Linearly Constrained Optimization

David M Gay, Bell Laboratories, New Jersey, USA

This paper suggests a class of trust-region algorithms for solving linearly constrained optimization problems. The algorithms use a "local" active-set strategy to select the steps they try. This strategy is such that degeneracy and zero Lagrange multipliers do not slow convergence (to a first-order stationary point) and that no anti-zigzagging precautions are necessary. (Unfortunately, when there are zero Lagrange multipliers, convergence to a point failing to satisfy second-order necessary conditions remains possible.) We discuss specialization of the algorithms to the case of simple bounds on the variables and report preliminary computational experience.

Multigrid Methods for Problems with a Small Parameter

P W Hemker, Mathematical Centre, Amsterdam

We discuss problems related with the multigrid (MG-) solution of elliptic PDEs, in which the coefficient of the highest derivative contains a small

parameter. For the equation in two dimensions we consider discretizations of finite element type and for the solution of the resulting discrete systems we study possible variants of the MG-method. The purpose is to find robust variants, i.e. variants that -without modification- are applicable to a large class of PDEs. As special cases of our PDE we consider the anisotropic-diffusion and the convection-diffusion equation.

For the convection-diffusion equation the use of an asymmetric restriction is investigated, in particular in combination with the streamline-upwind Petrov-Galerkin discretization. A relation is given between the choice of the artificial streamline-upwind parameter and the choice of the asymmetric restriction in the MG-algorithm.

An MG-algorithm with the Incomplete Line LU-decomposition (ILLU) relaxation and a coarse grid correction with a (possibly asymmetric) Galerkin coarse grid discretization appears to be a suitable choice for all problems considered.

Nonconvex Minimization Calculations and the Conjugate Gradient Method

M J D Powell, University of Cambridge

The conjugate gradient method is highly useful for the unconstrained minimization of functions of many variables, but most convergence theory does not apply to nonconvex objective functions that are continuously differentiable and that have bounded level sets. We consider this important class of problems, assuming exact arithmetic and exact line searches. Unfortunately we find examples that show that the calculated gradients can remain bounded away from zero. The examples that have only two variables show also that variable metric algorithms for unconstrained optimization need not converge.

Particle Approximation of Hyperbolic Equations

P A Raviart, Université Pierre et Marie Curie, Paris VI

Consider the Cauchy problem for an hyperbolic equation written in conservation form

$$(1) \quad \begin{cases} \frac{\partial u}{\partial t} + \sum_{i=1}^n \frac{\partial}{\partial x_i} (a_i u) + a_0 u = 0, & x \in \mathbb{R}^n, t > 0, \\ u(x, 0) = u_0(x). \end{cases}$$

A particle approximation u_h^0 of the solution u of Problem (1) is obtained as follows. We approximate the initial condition u_0 by a linear combination of Dirac measures

$$u_h^0 = \sum_j \alpha_j \delta(x - x_j).$$

Then, we define u_h to be the solution of (1) when replacing u_0 by u_h^0 .

This lecture will be devoted to the numerical analysis of the particle method: convergence and error estimates. Extensions of the method including the numerical treatment of boundary conditions and of diffusion terms will be briefly discussed.

Global Error Estimation for Stiff ODEs

L F Shampine, Sandia National Laboratories, USA

Numerical Techniques for Nonlinear Multi-Parameter Problems

A Spence, University of Bath

We consider nonlinear problems depending on parameters of the form

$$F(u, \lambda, \alpha) = 0, \quad F: \mathbb{R}^n \times \mathbb{R} \times \mathbb{R}^p \rightarrow \mathbb{R}^n,$$

where $u \in \mathbb{R}^n$ is a state variable, $\lambda \in \mathbb{R}$ a distinguished parameter, and $\alpha \in \mathbb{R}^p$ some auxiliary parameters. Such problems arise in many physical situations and usually one is interested in computing special values of the parameters, called "critical" values, at which the character of the solution changes. For example one may have buckling, spontaneous ignition, or the onset of instability, depending on the system studied.

Some examples will be given which illustrate the types of behaviour which may arise, and possible numerical difficulties will be discussed. Numerical techniques for the stable calculation of critical points or paths of critical points will be introduced.

Sequential Defect Corrections for High Precision Floating Point Computations

Hans J Stetter, Vienna, Austria

Recently, algorithms have been proposed and implemented which permit the computational solution of standard algebraic problems "without round-off", i.e. such that the approximate result computed in a floating point arithmetic is a pair of neighboring machine numbers which enclose the mathematically defined result. However, it has not become clear how these results are to be used as data in further algorithms of this type such that the final computational result of the sequence of algorithms achieves the same one bit accuracy.

After a discussion of the structure of these high precision algorithms, we shall establish the mechanisms which permit the transfer of suitable information from one algorithm to the next one such that their sequence may become a high precision algorithm itself. Possible uses and limitations of this approach will be discussed as well as implementation questions.

Numerical Experiments with Partially Separable Optimization Problems

Ph L Toint; A Griewank, Facultes Universitaires de Namur, Belgium

In this paper, we present some numerical experiments with an algorithm that uses the partial separability of an optimization problem. This research is motivated by the very large number of minimization problems in many variables having that particular property. The results discussed in the paper cover both unconstrained and bound constrained cases, as well as numerical estimation of gradient vectors. It is shown that exploiting the present underlying structure can lead to efficient algorithms, especially when the problem dimension is large.

The Numerical Solution of Total l_p Approximation Problems

G A Watson, University of Dundee

In many data fitting problems, there are errors in the $m \times n$ data matrix A as well as in the observation vector $b \in \mathbb{R}^m$. Some account can be taken of this by formulating and solving the total approximation problem of

minimising some norm of the $m \times (n+1)$ error matrix. For example the total least squares problem has attracted interest for many years, and has now been thoroughly investigated. Attention here is focussed on l_p norms, $1 \leq p \leq 2$. It is known that such problems are members of a class which may be solved through the solution of a vector norm minimisation problem in R^n with a single equality constraint. Numerical methods for such problems are considered.

An Implicit Diffusive Numerical Procedure for a Slightly Compressible Miscible Displacement Problem

Mary Fanett Wheeler; T C Potempa, Rice University, Texas

An implicit diffusive procedure is defined for computing the mole fraction distribution in a slightly compressible multicomponent single phase miscible displacement problem in a porous medium. Both a theoretical analysis and numerical results for this procedure are presented.

Singularities in Three-Dimensional Elliptic Problems and their Treatment with Finite Element Methods

J R Whiteman, Brunel University

In recent years mathematicians have produced finite element techniques with associated error analysis for certain elliptic problems involving boundary singularities; in the main two-dimensional Poisson problems. These theoretical techniques rely heavily on analytical results concerning forms of singularities and regularity properties of the solutions of singular problems. The availability of many such results for two-dimensional Poisson problems explains the attraction to this type of problem. Simultaneously engineers have created special elements and methods which produce accurate approximations to the solutions of three-dimensional elasticity problems containing singularities. This work has been motivated by the practical importance of linear elastic fracture mechanics and the methods are effective in applications for which linear elastic fracture is appropriate.

In the context of singularities there thus exists a considerable gulf between the area for which theoretical finite element analysis exists and those areas for which the finite element method is effective in engineering practice. This lecture describes work undertaken to try to close the gap. Knowledge of the form of the singularities is fundamental to the successful finite element treatment of singular problems. Therefore the forms of singularities in some three-dimensional Poisson and linear elasticity problems are first discussed. Ways of incorporating this knowledge into finite element methods are presented and analysed and their numerical performance is illustrated for various three-dimensional problems containing line singularities.

SECTION B

An Investigation into the Stability Properties of Second Derivative Methods with Perfect Square Iteration Matrices

C A Addison; P M Hanson, University of Victoria

We investigate the absolute stability properties of numerical methods for initial value O.D.E's using second derivative formulas where the regular iteration matrix, which is of the form $(I - b_0J - h^2c_0J^2)$, is approximated by a perfect square matrix of the form $(aI - hbJ)^2$. For the problem $y' = \lambda y$ we show that the region of stability depends not only upon the underlying formula, but also depends on the number of iterations and the predictor formula used. In particular, we show that the third and fourth order formulas used in BSLODE, and implementation of the blended formulas of Skeel and Kong (1977), are not A-stable unless three or more iterations are performed.

The calculation of free surface flows using a conformal transformation and boundary element techniques.

Joyce M Aitchison, University of Oxford

A novel method for the calculation of the time-dependent free surface problems of Hele-Shaw flow with suction and Saffman-Taylor channel flow is presented. The unknown fluid region is mapped conformally onto a unit disc, the free surface being mapped onto the unit circle. The mapping which is a function of time is calculated numerically using a form of the boundary integral method. Thus the free boundary position is found without explicitly calculating the pressure at all internal points.

The solution of these problems provides a non-standard application of the boundary element technique. Firstly the boundary of the region is exactly circular and the use of elements which are exactly circular arcs is demonstrated. These are found to be more straightforward to use than the conventional polygonal approximations. Secondly, the partial differential equations which are to be solved have associated auxiliary conditions in addition to the usual boundary conditions.

Numerical results are compared with the analytic solutions for various standard test problems. It is found that solutions to these unstable problems can be found for longer time periods than by using other methods, and that the computation times are significantly less since the solution is only calculated at boundary points.

A Comparison between Boundary Element Methods for the Acoustic Radiation Problem.

S Amini; D T Wilton, Plymouth Polytechnic

The exterior Helmholtz equation is commonly solved by Boundary Integral Formulations. Such integral equations however, when obtained by representing the solution as a single or a double layer potential or via Green's Theorem, suffer from lack of existence and uniqueness of a solution, for an infinite set of wavenumbers. There are boundary integral formulations valid for all wavenumbers but these are considerably more complicated. Here we shall implement and compare two such formulations, due to Panich and Burton and Miller.

Such problems are solved in a finite element fashion where low order polynomials are commonly used for the representation of the solution over each element. It is not in general clear whether the time spent in developing a complicated code which employs high order approximation of the unknown, is time wisely spent. Here we shall try and answer this question by comparing the results obtained using different orders of the approximating polynomials, for a range of test problems.

On Step Size Control for Volterra Integral Equations

H Arndt, University of Bonn

In numerically solving Volterra integral equations of the second kind

$$y(x) = g(x) + \int_a^x K(x,t,y(t))dt, \quad x \in [a,b],$$

where g and kernel K are given functions, known step size strategies proceed in the same way as in the case of ordinary differential equations.

Since for integral equations the integration is carried out over a triangle, such a step size control estimates the local error along the diagonal of the triangle only. We develop a step size policy that controls the local error over the whole triangle and demonstrate the efficiency of the modified step size control by examples.

Collocation Methods for Singular Perturbation Problems

Uri Ascher, Weizmann Institute, Israel

Singular perturbation problems for boundary valued ODEs are considered. For the numerical solution, high order symmetric and one-sided difference schemes, which are equivalent to certain collocation schemes, are applied. Experience with a general purpose collocation code on a variety of practical problems indicates that, while symmetric collocation can be successful in solving problems of this type, the convergence properties are different than usual.

To understand better the demonstrated performance of the numerical methods involved, we then analyze them carefully for a more restricted class of problems. For this class, it is shown that highly accurate solutions can be obtained at a very reasonable cost, using certain symmetric collocation schemes with appropriate meshes, whose construction is prescribed.

Recursive Calculation of Curved Finite Element Stiffness Matrices

M L Baart, NRIMS-CSIR, South Africa

A method is proposed for the evaluation of integrals that occur in the calculation of stiffness matrices when isoparametric or high order transformation bases are used on finite elements with curved sides. The propagation of errors in the initial values for the various forms of recursion is analysed. Several factors involved in the selection of a suitable recursion technique are discussed. Numerical results indicate that recursion can be used successfully even for those values of the parameters for which numerical instability in the evaluation of the analytic forms of the integrals would normally necessitate the use of cubature techniques.

A Multigrid Finite Element Method for General Regions

K Barrett, Coventry Polytechnic

The multigrid procedure has become an extremely popular method for solving elliptic boundary value problems since the pioneering work of Brandt in 1977. A robust computer package based on a finite element version of this technique with incomplete Choleski decomposition has been developed for a range of applications including steady heat flow, transonic flows in ducts and plane strain and stress and axisymmetric stress problems on simply connected regions. The heat flow examples are currently solved at the rate of 3000 unknowns/second of IBM 360/195 CPU time.

Higher order elements may be incorporated by using iterative schemes driven by the linear element approximations.

Work is in progress on extending the procedures to periodic problems.

Generalized Alternating Polynomials, Some Properties and Numerical Applications

L Brutman, University of Haifa, Israel

In the present paper we introduce the generalized alternating polynomials $A_n(x) = \sum_{k=0}^n a_k x_k^k$, the coefficients of which $a_0, a_1, \dots, a_n$ are defined together with L_n from the following linear system:

$$f(x_k) - A_n(x_k) = L_n T_{n+1}(x_k), \quad k = 0, 1, \dots, n+1,$$

where $T_n(x) = \cos(n \arccos x)$, $\{x_k\}_{k=0}^{n+1}$ - are $(n+2)$ distinct points in the interval $[-1, 1]$ and $f(x)$ is a continuous function on $[-1, 1]$. For the set of nodes $x_k = \cos[k\pi/(n+1)]$ $A_n(x)$ coincide with the polynomials of equiamplitude alternation introduced by de La Vallée-Poussin and discussed in the literature earlier (Eterman, Malozemov, Meinardus, Cheney and Rivlin, Brutman and others).

It is shown that the generalized alternating polynomials are related to the polynomials of interpolation by the Lanczos economization process and some of their approximation properties are formulated.

Several numerical applications of the A_n -polynomials are discussed, such as an effective evaluation of the remainder term of quadratures and numerical solution of algebraic and integral equations. The effectiveness of the alternating polynomials in applications is due to the presence of a parameter L_n which is a reasonable estimator of the error in the numerical solution.

Unconstrained Optimization by Approximation of the Gradient Path.

J P Bulteau, Université Catholique de Louvain, Belgium.

In the classical unconstrained minimization methods, the search for a new iterate is performed from the current point along a straight half line. This search direction should satisfy contradictory requirements. Far from the optimum or if the second order approximation of the function to be minimized is not relevant, the gradient direction should be preferred. For a better second order approximation and near the optimum, the Newton (or quasi Newton) direction becomes very useful. Methods have been devised to achieve such a compromise : dog-leg (Powell, Dennis and Mei), gradient path approximation (Botsaris, Vial and Zang) or trust region methods (Powell, Sorensen).

These methods, in particular gradient path and trust regions appear to be very powerful in terms of function evaluations. Their common drawback, however, is the sizeable amount of work which is required to compute the coordinates of the points of the curvilinear arc along which the one dimensional search is performed.

The method we propose overcomes this difficulty by performing the line search along an arc which shares with the gradient path of Vial and Zang its main features and considerably reduces the computational cost.

Successor points along this so simplified arc are chosen by using a trust region scheme.

We prove global convergence of our method, asymptotic quadratic convergence in the Newton case and Q-superlinear convergence with a quasi-Newton scheme.

ODE Solvers for Trajectory Problems and Applications to PDES

P Camino; J M Sanz-Serna*, *Universidad de Valladolid, Spain

J Lambert and R McLeod presented at the 1979 Dundee conference a method for the numerical treatment of differential equations $dy/dt = F(y)$ in situations where the interest lies in 'drawing' the trajectory of the solution rather than in finding the correspondence between points on the trajectory and values of t . We shall present several multistep methods for handling this sort of problem. We analyze the Lambert McLeod and the new methods and compare them numerically with some standard ODE solvers. Finally the Lambert McLeod scheme will be applied to the integration in time of semidiscretization of PDEs. This scheme is explicit and yet can conserve exactly quadratic quantities so that it is not subject to nonlinear blow-ups.

Spectral Solution of Stiff Piecewise-linear Differential Equations Occurring in Heat Transfer through a Network.

Cyril Carter, Trent University, Canada

The classical solution of a set of first order linear differential equations, as a spectral expansion in the eigenmodes of the coefficient matrix, is not a general practical computational may be in some circumstances. This paper considers the spectral solution of a certain class of stiff linear equations occurring in heat transfer through a network.

Given a network with N nodes, T and Q are the N -dimensional temperature and heat-source vectors, C is the positive diagonal thermal capacity matrix, G is the symmetric positive definite heat transfer matrix, with spectral radius $O(N^2)$. The differential equations to be solved are

$$CT(t) = Q(t) - GT(t) \quad (1)$$

The difficulty in solving these equations numerically stems from the very rapidly decaying transients arising from the larger generalised eigenvalues of G . Define a diagonal matrix D , with the eigenvalues in increasing order as its elements. Define a matrix X whose columns are the generalised eigenvectors, so that $GX = CXD$ with orthonormality relation, $X^T CX = I$. In terms of D and X , $G = CXDX^T$, $G^{-1} = XD^{-1}X^T$.

Define a diagonal exponential decay matrix, $E(t)$, with elements,

$\exp(-d_k t)$. The differential equations (1) may be transformed from nodal space into spectral (or modal) space by premultiplying with X^T . Then $X^T \dot{C}T = X^T \dot{Q} - DX^T CT$, a set of uncoupled differential equations in $X^T CT$, with solutions,

$$T(t) = XE(t)X^T CT(0) + XE(t) \int_0^t E^{-1}(t')X^T Q(t')dt' \quad (2)$$

The utility of this solution depends on the form of $Q(t)$, and the length of time over which the solution is valid.

Numerical evaluation of the complete spectrum requires $O(5N^3/3)$ arithmetic operations, about 10 times that needed for the symmetric triangular factorisation involved in an implicit finite difference solution of (1). However, the spectral solution (2) will often be valid over a much larger time interval than that needed for an accurate finite difference solution, and this may more than compensate for the extra arithmetic required to compute the complete spectrum for values of N up to several hundred.

Another interesting possibility being investigated is the use of a partial spectrum, in which the smaller elements of $E(t)$, arising from the larger eigenvalues, are neglected.

The Calculation of Directions of Negative Curvature for Non-linear Minimization Problems

A R Conn; N I M Gould*, *University of Waterloo, Canada.

Many algorithms for constrained optimization require directions of negative curvature.

We motivate and present methods that are particularly appropriate when applied to problems for which the expected number of active constraints is small.

Algebraic Stability for Explicit Runge-Kutta Methods

G J Cooper, University of Sussex

Nonlinear stability studies use a monotonic test problem. The scope of these studies can be widened by adding a boundedness property to this problem. This gives a more general definition of algebraic stability and leads to useful results for explicit, as well as implicit, methods.

Piecewise Monotonic Least Squares Data Fitting

I C Demetriou, University of Cambridge

This paper is concerned with the development of some efficient algorithms for making the smallest changes to measured data so that the final values are consistent with an underlying function whose first derivative changes sign at most a prescribed number of times. The main difficulty of this calculation is that the optimal positions of the sign changes have to be found automatically, but so many likely combinations of extrema can occur that it is impossible to test each one. In addition, a general optimization algorithm can terminate at a local minimum even if it is not an optimal solution. However, when the approximation is required to minimize the sum of squares of changes to n data subject to the above-mentioned conditions, the following idea from Dynamic Programming

may be used to calculate the optimal solution with q extrema. Let $r(k,i)$ be the least sum of squares of data changes that give a fit to the first i data with k extrema.

Then, $r(k,i) = r(k-1,j) + m(j+1,i)$, where $m(j+1,i)$ is the sum of squares of residuals of a monotonic fit to data whose indices are $j+1, j+2, \dots, i$, and where j is found to minimize $r(k,i)$. Thus, the complete calculation requires only of order qn^2 operations. Further saving can be obtained from the fact that the optimal j is a monotonically increasing function of i .

Numerical Scheme for a Groundwater Flow Problem with Radionuclide Seepage D B Duncan, Chalk River Nuclear Labs., Canada

A mathematical description of radionuclide seepage in groundwater flowing through soil has the following form in one space dimension

$$\frac{\partial c}{\partial t} + \frac{\partial S(c)}{\partial t} + V \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2}$$

where c is the concentration of radionuclide in the water, V is the water velocity, D is the diffusion coefficient and $S(c)$ is a specified function. $\partial S/\partial t$ represents the absorption rate of the nuclide onto the surface of the soil particles.

We examine some numerical approximations of this equation and consider their relationship to the physics of the problem. If dS/dc becomes unbounded (usually at $c=0$), numerical solution becomes more complicated. Other properties of the function $S(c)$ may also constrain the numerical scheme.

A simple numerical procedure is presented which avoids some of the more common difficulties.

Ordinary Differential Inclusions and Equations with Discontinuous Right Hand Sides

C M Elliott, Imperial College, London

Two problems are considered:-

$$(1) \quad -\frac{dy}{dt} \in \beta(y) - f(t,y), \quad y(0) = y_0$$

$$y \in H \equiv \{\mathbb{R}^n, \langle \cdot, \cdot \rangle\}$$

where $\beta(\cdot)$ is a multi-valued maximal monotone mapping on H .

Under certain conditions the backward Euler and implicit midpoint methods are shown to be convergent with an error bounded by a constant times the step length.

$$\begin{aligned}
 (2) \quad \frac{dy}{dt} &= f^-(t, y) & G(y) < 0 \\
 &= f^+(t, y) & G(y) > 0 \\
 &= ? & G(y) = 0
 \end{aligned}$$

$$y(0) = y_0, \quad y \in \mathbb{R}^n, \quad G: \mathbb{R}^n \rightarrow \mathbb{R}$$

An explicit one step method for computing sliding solutions, i.e. $G(y) = 0 \quad \forall t \in [t_1, t_2]$, will be presented.

Implicit Multistage Methods for Ordinary Differential Equations and their Efficient Implementation

Roland England, IIMAS, Universidad Nacional Autonoma de Mexico

Butcher has considered implementing implicit Runge-Kutta methods by transforming the coefficient matrix B to diagonal form, PBQ , where PQ is lower bidiagonal. He thus reduces the cost of the matrix operations, and could also do so for any method of his class (A, B, C)

$$y_i^{(n)} = \sum_{j=1}^s \{ a_{ij} y_j^{(n-1)} + h b_{ij} f(y_j^{(n)}) + h c_{ij} f(y_j^{(n-1)}) \}.$$

To facilitate changing of the step size h , without completely refactorizing the iteration matrix, Enright has proposed a transformation of the Jacobian matrix $J = \partial f / \partial y$ to upper Hessenberg form $L^{-1} J L$, where L is lower triangular. These two ideas may be combined for further efficiency, but further economies are possible when B has a pair of complex eigenvalues, as for the author's hybrid implicit methods, of the form:

1. an interpolation formula

$$y_{n+\theta} = \sum_{j=0}^k (\alpha_j y_{n+1-j} + \beta_j h \dot{y}_{n+1-j})$$

2. a quadrature formula

$$y_{n+1} - y_n = h \sum_{j=0}^k \gamma_j \dot{y}_{n+1-j} + h \delta f(y_{n+\theta}).$$

The same problem arises for Skeel and Kong's Blended Multistep Methods, for which they approximate a quadratic form in J by a perfect square, and reduce the rate of convergence. When implementing Enright's Second Derivative Multistep Methods, Addison has proposed combining this approximation with the Hessenberg transformation. Here, it is shown that it is usually more efficient to use the exact quadratic form, particularly

when combined in a new way with the Hessenberg transformation.

On the Lacunary Interpolation with Splines

Th Fawzy; I Refat^{*} (1), ^{*}Salmiya, Kuwait

A new method for solving the $(0,1,3)$ interpolation problem with spline functions is presented. It has been shown that if $f \in C^{(r)}[a,b]$, $r = 3, 4$ and 5 , $f \in \text{Lip}_M^\alpha$, then the error is $O(h^{r+\alpha-1})$ in $f^{(i)}(x)$ where $i = 0, 1, \dots, r$ and $0 < \alpha \leq 1$. The stability of such interpolation is also investigated.

On the Approximate Solution of the D E $y'' = f(x, y, y')$

Th Fawzy ; I Refat (2), ^{*}Suez Canal University, Egypt

A new method for approximating the solution of the initial value problem $y'' = f(x, y, y')$ with spline functions is presented. The spline function approximating the solution is not necessarily polynomial spline. It is a one-step method $O(h^{2+\alpha})$ in $y(x)$, $y'(x)$ and $y''(x)$ where $f \in C([a,b] \times \mathbb{R}^2)$, $f \in \text{Lip}_M^\alpha$ and $0 < \alpha \leq 1$.

Expected Conditioning

R Fletcher, University of Dundee

A perturbation analysis based on probabilistic arguments is developed for a range of problems in numerical linear algebra, and this talk concentrates on the case of a well determined linear system. Condition matrices and condition numbers are determined for the expected value of the actual conditioning of a problem. These enable attainable lower and upper bounds on the expected condition number of a matrix to be given, independent of any particular linear system. These estimates are much more reliable than those derived from conventional norm condition numbers and are shown to reveal features which the latter cannot.

The expected condition analysis has desirable properties under scaling transformations which is not the case for the norm condition analysis. It is shown that an optimal (or natural) scaling can be associated with any matrix and is readily computed. This enables the equilibration of a matrix to be carried out. Because this process is a uniquely defined projection, it always enables the best possible of all possible equilibrated matrices to be determined.

A report NA/63 is available on request.

Stable Modification of Explicit LU Factors for Simplex Updates

R Fletcher; S P J Mathews, University of Dundee

This paper presents a method for modifying an LU factorization of a matrix A when a Simplex update is performed on A. At each stage of the algorithm two options are allowed, and in one of these a row permutation of L is made so that the LU structure is always maintained. The expanding file of operators used in other methods is not required. The result of an error analysis is presented in which the error is bounded by the growth in the partial sums of LU. Various pivotal strategies which minimize a growth bound are discussed and an example is given for which the maximum growth is attained. Numerical experiments on ill-conditioned problems show no tendency for error growth. A report NA/64 is available on request.

An Improved Newtons' Method

M Friedman ; G Erez, * Nuclear Research Center - Negev, Israel

The standard Newtons' iterative method for solving $F(X) = 0$, converges quadratically. It can be improved to guarantee cubic convergence provided that some additional function computations are performed. Further improvements are also possible by replacing derivatives with their finite differences equivalents. In this work the original scheme is modified so that less function evaluations are needed to achieve the same quadratic rate of convergence.

Methods for Ordinary Differential Equations with Discontinuities

C W Gear; O Osterby, * University of Aarhus, Denmark

Many problems in simulation and control give rise to systems of ordinary differential equations $y' = f(x, y)$ in which the right-hand-side function f contains discontinuities in the form of finite jumps either in components of f itself or in some derivatives of f . Numerical software for solving ODEs will often behave very inefficiently in the presence of such singularities and it is the aim of this paper to show how these shortcomings can be remedied.

We distinguish between four computational stages and shall treat each of them in detail:

1. Detecting the possible presence of a discontinuity. This should be a very low cost set of tests because it must be activated at every rejected step of the integration routine.
2. Locating the discontinuity. After the presence of a discontinuity is detected we must find the location of it as quickly and efficiently as possible.
3. Passing the discontinuity. When we know where the discontinuity is we can step right up to it and step across it with due regard to the size of the local error involved in the crossing.
4. Restarting. Since the previous values of y and f no longer correspond to smooth functions we must be careful with using such information. The restarting procedure must be chosen according to the nature of the discontinuity.

A Filled Function Method for Finding the Global Minimizer

Ge Renpu, Xi'an Jiaotong University, China and University of Cambridge

The concepts of filled function and generalized filled function are introduced. Two such functions are

$$P(\underline{x}, r, \rho) = F(\underline{x}) + r \exp(-\|\underline{x} - \underline{x}_j^*\|^2 / \rho^2) \quad (1)$$

$$\tilde{P}(\underline{x}, r, \rho) = \exp(-\|\underline{x} - \underline{x}_j^*\|^2 / \rho^2) / [\hat{r} + F(\underline{x})] \quad (2)$$

where $r, \rho, \hat{\rho}$, are positive constants, r is a constant but may be negative,

$F(x)$ is the objective function, x_1^* is a minimizer of $F(x)$, which has been located. The properties of functions (1) and (2) are analysed. They have a maximum at x_1^* and a hill covering the basin of x_1^* and they have minimizers from which one can minimize $F(x)$ to find other minimizers of $F(x)$. If one only uses the second one, when ρ is sufficiently small, only the lower minimum points of $F(x)$ can be located. Therefore one can make sure that a global minimizer has been located and terminate the computation provided one can find a region outside which there is no minimizers of $F(x)$ at all. Six functions, including 6-hump back camel function, Branin function and Goldstein and Price function, have been tested successfully by using combinations of (1) and (2) or only (2) in a short time starting with an arbitrary initial point.

Accurate Boundary Treatment in Shallow Water Flow Computations

Herman Gerritsen, Delft Hydraulics Laboratory, The Netherlands

The shallow water equations are a model for the description of horizontal flow in shallow areas such as lakes, rivers, coastal seas, etc. Characteristic of the computational region in all practical applications is the presence of both closed boundaries (no throughflow) and open boundaries (non-physical, free throughflow). At these boundaries boundary conditions are applied to determine a physically realistic and unique solution in the interior part of the area under consideration.

In many computations disturbances occur. Stability is then retained by means of addition of extra bottom friction, diffusion or smoothing operations. This is an undesirable procedure, however.

The disturbance and instabilities mentioned are often the result of unsatisfactory modelling, especially at the boundaries. One should therefore try to improve the boundary treatment.

In this paper a method for the treatment of closed boundaries is presented. Locally the equations for the derivatives in normal direction are introduced. This makes it possible to use central differences at the boundary in the same systematic way as this is done in the interior. It also avoids the introduction of extraneous numerical boundary conditions. Consequently, the generation of high frequency disturbances resulting from discontinuities in the truncation errors is minimized. Optimal use of the boundary equation $u_n = 0$ and the local field equations results in the correct wave reflection, independent of the angle of incidence of the waves.

This approach is also followed at open boundaries both when velocities, or when ingoing Riemann invariants are prescribed.

In a number of numerical experiments the boundary treatment has been tested. To do so, the implicit fully second order accurate neutrally stable scheme of Briley and MacDonald was chosen. The equations were then solved after application of an ADI-splitting technique.

The results justify the conclusion that the systematic and identical second order treatment of all computational points with central differences leads to higher global accuracy and enhances stability.

The Double Secant Method for Real Polynomial Equations

J K Gibson, Birkbeck College, London

A method, similar to Bairstow's method, for finding a real quadratic factor of a real polynomial, may be derived from Newton's method in the following way.

Let (a_n) and (b_n) be sequences of Newton iterates converging to the roots a and b of the polynomial P , and let $F_n = x^2 + A_n x + B_n$ have roots a_n and b_n . It is not difficult to construct an iterative algorithm to compute the sequences (A_n) and (B_n) converging to A and B . Then $F = x^2 + Ax + B$ is either a quadratic factor of P , or the square of a linear factor.

The algorithm, like Bairstow's, requires little more than division of P by F_n to produce a quotient Q_n and a remainder R_n , and then division of Q_n by F_n to produce a remainder S_n . Convergence is quadratic if a and b are simple roots of P .

Such a method may be called the Double Newton method. It has no advantage over Bairstow's method, and as it stands suffers from three disadvantages:

1. When a is a simple real root of P , it will often happen that $b = a$, and then F is only the square of a linear factor of P .
2. Even when (a_n) converges, (b_n) may diverge, or converge much more slowly than (a_n) .
3. If a_1 and b_1 are real, then a and b must be real.

However, a similar treatment may be applied to the Secant method to obtain a Double Secant method. At little extra cost the disadvantages of the Double Newton method may be overcome, and the resulting algorithm has two advantages over Bairstow's method:

1. Only one polynomial division is required for each iteration.
2. Convergence from an arbitrary starting point is more likely.

The Double Secant method has been used successfully to find all roots of polynomials, both with a Fortran program, and with a multiprecision program written in Z80 assembler. Results indicate that convergence depends primarily on whether the polynomial is well enough behaved for the precision used, and does not depend much on the starting point used. Convergence seems almost quadratic for simple roots.

Implementation of Second Derivative Methods for Implicit Second Order Systems

I Gladwell*, C A Addison, *University of Manchester

We demonstrate a technique for implementing the second derivative methods of Enright for implicit initial value problems,

$$M\dot{y} + Cy + Ky = f(t), \quad y(0) = y_0,$$

in such a way as to factorise only a single matrix of the form $(M + h r C + h^2 r^2 K)P$ for any given stepsize h . We discuss the efficiency of using a class of formulae for which r is complex and $p = 1$, in comparison with others for which r is real and $p = 2$.

A Boundary Element Method for Computing 3-D Viscous Incompressible Fluid Flows

K Hebeker, University of Paderborn

Nowadays the numerical computation of 3-D viscous incompressible fluid flows is a main problem in mathematical physics, for the widely developed methods (FEM or FDM or spectral methods) lead to great practical complexity, or they are restricted to simple geometries. On the other hand boundary element methods lead to simple and efficient algorithms for viscous flows in smoothly bounded but otherwise arbitrary regions: besides the well-known advantages of boundary element methods the incompressibility constraint is automatically satisfied.

In the present lecture an ansatz with hydrodynamical potentials will be proposed for solving the 3-D exterior Stokes' boundary value problem. When applying the classical double-layer potential ansatz (Odqvist) the resulting integral equations' system is non-uniquely solvable, hence useless for numerical purposes. Hence here we propose a combined ansatz of a simple - and double - layer potential.

This approach leads to a Fredholm integral equations' system of the second kind which proves to be uniquely solvable, hence inducing attractive numerical algorithms.

This integral equations' system is discretized by a collocation procedure. Then we get the convergence theorem: the sequence of the approximate velocities in the exterior region uniformly and quadratically converges to the flow's exact velocity field.

Finally we will present numerical results of test computations when the linear system is solved by

- Jacobi and Gauss-Seidel iterations;
- a two-grid method;
- Gauss elimination.

A Moving-Grid Method for Tracking Shocks

G W Hedstrom, Lawrence Livermore National Laboratory, California

A method is presented for tracking shocks for nonlinear hyperbolic systems in $R^2 \times [0, T]$. A moving orthogonal grid based on Hermite cubic splines is used. An axisymmetric gas dynamics problem is used to illustrate the method. The computer program is designed to handle several shocks by using multiple grids, but it is currently being tested on a single shock.

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract No. W-7405-ENG-48.

Stability and the Nonlinear Schrodinger Equation

B M Herbst, University of the Orange Free State and University of Dundee

The numerical stability of the nonlinear Schrodinger equation will be discussed. In particular it will be shown that the low frequencies are unstable to small perturbations. It will also be shown that the "strength" of the nonlinearity can influence instability. Numerical examples of nonlinear instability will be given.

Upper Bounds for the Condition Number of a Triangular Matrix

N J Higham, University of Manchester

A technique is derived which enables cheap computation of an upper bound γ for $\|T^{-1}\|_{\infty}$ when T is a triangular matrix. It is shown that $\gamma/\|T^{-1}\|_{\infty} < 2^{n-1}$ for those matrices T which arise in the QR decomposition with column pivoting, $Q^T A P = \begin{bmatrix} T \\ 0 \end{bmatrix}$. From this decomposition, upper and lower bounds for $\text{cond}_2(A)$ are obtained.

SIL - a Simulation Language

Niels Houbak, Technical University of Denmark

SIL is an ALGOL-like simulation language designed for the solution of coupled systems of non-linear algebraic equations and ordinary differential equations, possibly containing discontinuities. In SIL, the system of algebraic equations is solved by the Newton method and we use STRIDE (Burrage, Butcher and Chipman) for the solution of the system of ODE's. SIL is primarily intended as a tool for education and research. The problems solved so far include the Van der Pool equation, root-locus problems from the stability analysis of Runge-Kutta methods, and simulation of chemical reactors as well as the on-off control of refrigerators.

Linear Multistep Methods with Minimized Truncation Error for Periodic Initial Value Problems

P J Van Der Houwen*, B P Sommeijer, *Mathematical Centre, Amsterdam

A common feature of most methods for numerically solving ODEs is that specific properties of the solution are not exploited by the method. Here we consider initial value problems the solution of which is a priori known to possess an oscillatory behaviour. The methods to be derived are of linear multistep type and special attention is paid to the minimization of those terms in the truncation error which correspond to the oscillating components. Numerical experiments are reported and compared with results obtained by conventional linear multistep methods and by the methods of Gautschi.

B-Stability for Semi-Implicit Methods

W H Hundsdorfer, University of Leiden, The Netherlands

We consider the initial value problem $U'(t) = f(U(t))$, $U(0) = u_0$, where $u_0 \in \mathbb{R}^S$ and $f: \mathbb{R}^S \rightarrow \mathbb{R}^S$ is dissipative and nonlinear. For the numerical solution we deal with semi-implicit methods (e.g. ROW-methods) yielding approximations u_n to $U(nh)$ that satisfy

$$u_{n+1} = u_n + \sum_{i=1}^m b_i (hJ(u_n)) h f(y_i)$$

$$y_i = u_n + \sum_{j=1}^{i-1} a_{ij} (hJ(u_n)) h f(y_j) \quad (1 \leq i \leq m)$$

Here $h > 0$ is the stepsize, the b_i and a_{ij} are rational functions, and $J(u_n) \approx f'(u_n)$.

If the solution $U(t)$ tends to a stationary solution, $U(t)$ becomes very smooth and the local error will permit a (rather) large stepsize.

In this talk we consider the question whether such a large stepsize will cause instability. Theoretical results will be presented for different

choices for $J(u_n)$ ($J(u_n) = f'(u_n)$, $f'(u_n + \text{chf}(u_n))$, and J is constant).

References

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2. Hairer, E., Bader, G., Lubich, Ch.: On the stability of semi-implicit methods for ordinary differential equations. BIT 22, 211-232 (1982).
3. Hundsdorfer, W.H: Nonlinear stability analysis for a simple Rosenbrock method. Report 81-31. Institute of Applied Mathematics and Computer Science, University of Leiden, 1981.

Order Stars and Finite Differences for Parabolic PDE's

A Iserles, King's College, University of Cambridge

Given the finite difference discretization

$$\sum_{j=-r}^r \alpha_j(\mu) u_{m+j}^{n+1} = \sum_{j=-r}^r \beta_j(\mu) u_{m+j}^n$$

$\mu = \omega \Delta t / (\Delta x)^2$, $r \geq 1$ of the differential equation $\mu_t = \omega u_{xx}$ we prove that a unique choice of coefficients gives order $4r+1$ and that no higher-order method exists. Furthermore, we show that for every $r \geq 1$ the highest-order

method is stable. Our proofs use order stars of first and second kinds, as well as the Pade approximation theory and computational complex analysis. The Crandall scheme with $r = 1$ and order 5 is the simplest example of the considered methods.

Numerical Solution of Continuous Chebyshev Approximation Problems

K Jonasson, University of Dundee

A globally convergent method is presented for the solution of problems of the form

$$\min_{\underline{a}} \| f(\cdot, \underline{a}) - g \|_{X, \infty}$$

where X is a (simple) compact set in $\mathbb{R}^n$ and $f: X \times \mathbb{R}^n \rightarrow \mathbb{R}$ and $g: X \rightarrow \mathbb{R}$ are twice continuously differentiable. The method is based on rewriting the problem locally as a minimax problem of the form $\min_a \max_i f_i(a)$ and solving quadratic programming subproblems. Some numerical results for the case $m = 2$ are given.

A Collocation Method for Singularly Perturbed Two-point Boundary Value Problems with a Turning Point

P E Koch, University of Oslo

Consider a linear, second order, singularly perturbed two-point boundary value problem with a turning point giving boundary layers. We approximate the solution by combinations of piecewise polynomials and piecewise exponentials. These approximations are determined by collocation at

Gaussian points. If the differential equation has smooth coefficients and right side, then for sufficiently stiff problems, the convergence will be of the same order as that of the polynomials used in each subinterval.

For example, consider the turning point problem,

$$-\epsilon x'' + tx' + \alpha x = f, \quad -1 \leq t \leq 1$$

$$x(-1) = 0, \quad x(1) = 0$$

where $0 < \epsilon \ll 1$ and $\alpha > 0$. We partition $[-1,1]$ into subintervals $I_i = [t_i, t_{i+1}]$ with one $t_j = 0$. As collocation points we may for instance choose the zeroes of the second degree Legendre polynomial relative to each I_i . On I_i we want the collocation approximation to be a linear combination of quadratic polynomials and ϕ_i , where

$$\phi_i(t) = \begin{cases} \exp(t_{i+1}(t-t_{i+1})/\epsilon), & t_i \geq 0 \\ \exp(t_i(t-t_i)/\epsilon), & t_i < 0 \end{cases}, \quad t \in I_i$$

If f is smooth then the collocation approximation will approximate the solution x with an error of $O((\max \Delta t_i)^3)$ on $[-1,1]$ as $\epsilon \rightarrow 0$.

Practical Error Estimates in Numerical Integration

D P Laurie, NRIMS-CSIR, Pretoria, South Africa

The error incurred by the use of a given interpolatory quadrature rule, compounded once, is estimated by the following procedure:

- Obtain an auxiliary interpolatory quadrature rule of lower degree than the original rule. (A natural way of obtaining such a rule is to drop a point from the given rule, and to calculate new weights for the remaining points. The error estimate given here is independent of the choice of the point to be dropped.)
- Calculate an improved value for the integral under the assumption that the auxiliary rule is effectively of the same degree as the original rule, by using nonlinear extrapolation. The error estimate is the difference between the improved value and the original compounded value.

Even though the assumption is often invalid, the estimate has two highly desirable properties:

- If both rules converge monotonically, and the more accurate rule converges faster when compounded, the estimate bounds the error, even when the assumption of equal degree fails.
- Although the "improved" value is in fact worse than the original compounded value when the equal degree assumption fails, the error estimate obtained is nevertheless much sharper than that obtained by merely using the difference between the original and auxiliary rules.

When this error estimate is used inside an adaptive quadrature routine, it

is necessary to have error estimates over each subinterval. A way of allocating the total error estimate over the subintervals is derived heuristically.

Numerical experiments show the effectiveness of the estimate on some existing automatic adaptive integrators.

Solution of Weighted Linear Least Squares Problems with Simple Structure
P E Manneback, University of Namur, Belgium and NPL Teddington

A numerical method of solution is considered for the problem of the least squares fitting of correlated experimental data. The introduction of a non-diagonal variance matrix V in the regression model implies extra computation and storage requirement compared with the classical uncorrelated model. This extra amount of work consists principally in finding the Cholesky factor L of V , and in solving the lower triangular system $LX = A$, where A is the observation matrix. We show that if V has a special structure, e.g. V is estimated by a rank one modification h of a diagonal matrix D ($V = D + hh^T$), the work can be considerably reduced. In fact, the problem can be solved by a row by row updating using Givens Rotations, as it is for a non-weighted regression.

The problem of fill-in in the substitution $LX = A$ is examined and an algorithm is described for finding a row permutation of A which reduces the fill-in occurring in solving this system. A special emphasis is made on spline fitting.

Bifurcation Studies in Reaction-Diffusion
V S Manoranjan, University of Dundee

The steady state solutions arising beyond a point of instability are studied for a nonlinear reaction-diffusion equation using simple numerical schemes. Comparisons are made with analytical results wherever possible.

L_p Approximation by Real and Complex Chebyshev Series
J C Mason, Royal Military College of Science, Shrivenham

For continuous functions, it is well known that the Chebyshev series projection provides a near-best approximation in the L norm. In fact this result extends not only to all L_p norms ($1 \leq p < \infty$) but also to a variety of real and complex function spaces, including analytic function spaces on elliptical domains and annuli. It is also well known that, in L , whereas the Fourier series projection is minimal on continuous periodic functions, the Chebyshev series projection is not minimal on continuous functions. This surprising result is clarified (in both real and complex variables) by considering two types of Fourier-Chebyshev projections, a "generalised Fourier-Chebyshev projection" which is minimal in all L_p norms, and an "even/odd Fourier-Chebyshev projection" which is not.

Stability Analysis of High Accuracy Methods for Fourth Order Parabolic Equations

E J W Ter Maten*, G L G Sleijpen, *University of Utrecht

Consider the fourth order parabolic partial differential equation (PDE):

$$u_{tt}(x,t) = - \sum_{j=1}^M a_j(x) \frac{\partial^4}{\partial x_j^4} u(x,t) \quad x \in \Omega \subseteq \mathbb{R}^M, \quad t \geq 0 \quad (+)$$

in which the a_j are positive functions. In addition to (+) u satisfies some boundary and initial value conditions.

For the case $\Omega \subseteq \mathbb{R}$ we consider finite difference methods for (+). These methods can be related to methods for a first order formulation of the above PDE:

$$v_t = \begin{bmatrix} 0 & -L \\ L' & 0 \end{bmatrix} v \quad \text{in which } L' := \frac{\partial^2}{\partial x_1^2} \text{ and } L := a_1 \frac{\partial^2}{\partial x_1^2}$$

Here the stability analysis of the methods concentrates on the first order forms. In the constant coefficient case many of these methods can be viewed to be rooted in Cayley transforms. Since any Cayley transform is unitary, in such a situation, the stability follows. The class of Cayley transforms is extended. Thus obtaining a way to analyse the stability of the above methods also in the case of variable coefficients and also for methods which have a high accuracy with respect to the spatial stepsize.

For the one-dimensional PDE (+) strong stability results are given. The profitable methods are used in high accuracy ADI-methods for more dimensional problems. For the constant coefficient case stability conditions for these ADI-methods are deduced.

Divided Differences and Defect Correction for the Finite Element Method

G Moore, National Institute for Higher Education, Dublin

Traditionally the justification for defect correction has rested on asymptotic expansions in powers of h (Pereyra, Stetter). Recently, however, Skeel (S.J.N.A., 1982) has suggested that smoothness requirements should be measured by norms based on divided differences, which provides a more natural setting for convergence results. We shall show how this type of analysis may be applied to simple examples of the finite element method.

A Global-Local Finite Element Method in Space-Time for a Convection - Diffusion Problem

F D Van Niekerk, University of Pretoria, South Africa

In this paper we discuss the numerical solution of the convection - diffusion equation

$$\frac{\partial u}{\partial \tau} = \varepsilon \frac{\partial^2 u}{\partial t^2} - \delta \frac{\partial u}{\partial x}, \quad \varepsilon > 0, \quad \delta > 0$$

on the strip $(x,t) \in (0,1) \times (0,\infty)$.

Basis functions in space and time are applied simultaneously, globally in space but locally with respect to time. This approach differs from the traditional finite element treatment. We consider three problems associated with this equation corresponding to the initial condition

$$u(x,0) = u_0(x), \quad x \in (0,1)$$

and the following boundary conditions:

1. Homogenous Dirichlet conditions
2. Periodic conditions
3. Neumann conditions.

We assume that convection dominates diffusion and that the initial data is a triangular pulse.

Numerical Methods for Solving Inverse Eigenvalue Problems

Jorge Nocedal^{*}; Michael Overton, ^{*}New York University

We investigate two numerical methods for solving inverse eigenvalue problems. They can be regarded as the application of Newton's method to two different formulations of the problem. We discuss convergence rates and stability and show that one of the methods is clearly superior to the other one. We describe several applications in nuclear physics, Sturm-Liouville problems and Factor Analysis. Finally, we prove that the good method has quadratic convergence even in the case of multiple eigenvalues. We discuss the implications of this result.

Two-Point-Boundary-Value Problems with Interval Analysis

F Aleixo De Oliveira, University of Coimbra, Portugal

Applying interval-analysis methods to the computation of an approximate solution, for a given two point boundary value problem $y'' = f(x,y,y')$, $y(a) = \alpha$, $y(b) = \beta$, we will achieve a related initial value problem $y'' = (x,y,y')$, $y(a) = \alpha$, $y'(a) \in c^1$, where c^1 is a real interval $[c,c]$. Solving that, again with an efficient initial value interval analysis method, we obtain arbitrary sharp bounds on the solution of the two point boundary value problem, for $x_i \in [a,b]$, $i = 0, \dots, n$.

With these and with an interval version of the cubic, interpolator, natural spline function, we obtain an interval-global solution for the given two point boundary value problem.

Richardson's Iteration for Nonsymmetric Matrices

Gerhard Opfer, University of Hamburg

Richardson's iteration is a method for solving the linear system $Ax = a$ by an iteration of the form

$$x_{j+1} = x_j - \alpha_j (Ax_j - a), \quad j = 1, 2, \dots$$

where the intelligent choice of the α 's is the main problem. For real, symmetric definite matrices this problem can be solved explicitly, cf. D Young's book, also for further references. For real, symmetric but indefinite matrices the problem was recently treated by de Boor & Rice (SIAM J. Sci. Statist. Comput. 3 (1982), 47-57). In the general case one has to solve the Chebyshev approximation problem: Minimize $\|1 - (a_1 z + a_2 z^2 + \dots + a_n z^n)\|_\infty$ on a set $S \supset \sigma(A)$ where $\sigma(A)$ is the spectrum of A. Theoretical and numerical results will be presented.

A Class of Methods for Stiff Ordinary Differential Equations

F Patricio, University of Coimbra, Portugal

A class of K-step methods suitable for the numerical integration of stiff systems of first-order ordinary differential equations is presented.

To get good conditions for the stability of the methods we fix the interval I_k of variation of the parameter V , for $k = 1, \dots, 6$. For $V \in I_k$ we get stiffly-stable formulae up to order 8 and A-stable formulae up to order 5. The maximum order achieved is $k+3$ and for $k \leq 5$ the methods are still stiffly-stable. For $k = 1, \dots, 6$ and $V \in I_k$ we give the stability parameters α , D [see C W Gear, Numerical Initial Value Problems in Ordinary Differential Equations, 1971]. Our class contains the methods of W H Enright [SIAM J Numer Anal., V. 11, 1974] and some of S Kovvali and G K Gupta [Math of Comp., V. 38, 1982]. Some numerical results are also discussed in the present paper.

Computing Square Roots with 15 Decimal Accuracy Using Only 4 Multiplications - and Some Algorithms

P W Pedersen, Technical University of Denmark

To compute $\sqrt{A}$ for A in the interval $I = [P, Q]$, let s denote an approximation

$$s := \text{APPROX}[\sqrt{A}]$$

Then x

$$x := A/s^2 - 1, \quad A = s^2(1+x) \quad (1)$$

will be close to zero and using the power series for $\sqrt{1+x}$ you get

$$\sqrt{A} : \approx s \cdot \left[1 + \frac{1}{2}x - \frac{1}{8}x^2 + \frac{1}{16}x^3 - \frac{5}{128}x^4 + \dots + c_p x^p \right] \quad (2)$$

For $p = 1$ you get the standard Heron-Newton formula of order 2. For p in general you get an approximation formula of order $p+1$.

The division in (1) can be avoided if you use as s a value s_i selected from the set

$$s_1, s_2, \dots, s_n \text{ in } SI := [\sqrt{P}, \sqrt{Q}]$$

for which you have stored $k_i := 1/(s_i)^2$.

Then $x := k_i A - 1$ and (2) will give $\sqrt{A}$ without division.

By arranging (2) in a suitable way some multiplications can be replaced by Shift- and Add multiplications with simple binary numbers (including s_i)

and for $p=6$ you can, with a reasonable number n , get 15 decimal accuracy in $[0.25,1]$ using only 4 normal (long) multiplications.

A Comparison of Numerical Methods for the Linear Generalized Abel Integral Equation

H J J te Riele; Philip Schroevers, *Mathematical Centre, Amsterdam

A comparison is made between a number of important representatives of the following classes of methods: (i) collocation -, (ii) product integration - and (iii) global methods, for the linear generalized Abel integral equation

$$\int_0^x K(x,t)f(t)(x-t)^{-\frac{1}{2}}dt = g(x), \quad 0 \leq x \leq X; \quad K \text{ and } g \text{ are given functions.}$$

Special attention is paid to the performance of these methods for problems with a non-smooth solution.

Vector Analogues of Aitken's δ^2 -Process

R A Sack*; R Brown, *University of Salford

This paper discusses and compares a number of analogues of the δ^2 process for the acceleration of multi-component iterative procedures. The optimal choice of method is strongly dependent on whether or not the iterations involve rotational component, i.e. whether the eigenvalues of the linearized iteration matrix are partly complex or all real.

These acceleration methods are applied to standard methods of solution of 2-dimensional PDE's, i.e. Jacobi, SOR, SSOR and checker-board. Accelerations by factors from 3 to 10 are obtained with a minimum of additional programming. For parallel processors a modification of the standard checker-board overrelaxation is proposed to eliminate complex eigenvalues; only one set of values is overrelaxed, the other set simply relaxed with a factor unity.

Finding the zeros of splines

Larry L Schumaker, Texas A&M University

In this paper we discuss the problem of numerically locating all zeros of a given B-spline series. One approach, of course, is to simply convert the spline to a piecewise polynomial and attack each piece with some polynomial root-finding scheme. Here we discuss some alternatives which seem to have advantages in some applications. Results of several numerical experiments will also be presented.

Optimal Error Estimates for Petrov-Galerkin Methods

B W Scotney, University of Reading

For diffusion-convection problems in which convection is dominant, Petrov-Galerkin methods are used to overcome the well-known inadequacies of the Galerkin method. The question arises as to how the test space should be chosen for a given trial space. We consider a factorisation of the differential operator which leads to the possibility of generating test spaces with a view to either producing a nodally accurate solution or a solution which is a best fit in a mixed norm. The Riesz Representation Theorem guarantees the existence of such spaces, and enables the relationship between the trial space - test space pairing and the

optimality of the associated Petrov-Galerkin method to be investigated. In particular for the one dimensional diffusion-convection problem we establish explicit optimal error estimates for any conforming 'upwind' finite element method when a piecewise linear trial space is used, and our framework is exploited to analyse the commonly used test spaces.

An Extension of a Theorem of J L Walsh
A Sharma, University of Edmonton, Canada

Recently Rivlin[1] extended a beautiful theorem of Walsh: if $f \in A_p, \rho > 1$ (the class of functions analytic in $|z| < \rho$, but not in $|z| < \bar{\rho}$), let $S_n(z)$ denote its Taylor polynomial of degree n . If $m = nq + c$, $0 < c < n$, let $P_n(z)$ denote the polynomial of degree n which minimizes $\sum_{k=0}^{m-1} |Q_n(w^k) - g(w^k)|^2$, ($w^n = 1$), over all polynomials of degree n . Rivlin showed that $\lim [P_n(z) - S_n(z)] = 0$ for $|z| < \rho^{1+q}$. For $m = n$, this gives the theorem of Walsh. The object here is to give a survey of some of the original literature related to it and to give some further extensions of this result.

1. T J Rivlin, On Walsh Equi-convergence. J Approx Theory, 36, 34-345, 1982.

Construction of Generalized Adams Methods for Stiff ODES
S Sigurdsson, University of Iceland

The following reformulation of the initial value problem:

$$y' = Ay + f(t, y) - Ay$$

results in the relation:

$$y_{n+1} = e^{hA} y_n + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-t)A} (f-Ay) dt, \quad h = t_{n+1} - t_n \quad (*)$$

a well-known starting point for obtaining modifications of Adams methods, suitable for stiff systems, that was originally (?) proposed by Certaine (1960). Typically e^{hA} is replaced by a rational approximation $O(hA)^{-1} P(hA)$ and $[f-Ay]$ by an interpolating polynomial. If $A = f/y$ (*) reduces to $y_{n+1} = Q^{-1} P y_n$ when applied to the linear system $y' = Ay$.

Multistep methods, in general, reduce however to a multistep expression of the form

$$y_{n+1} = Q(hA)^{-1} [P_0(hA) y_n + P_1(hA) y_{n-1} + \dots + P_K(hA) y_{n-K}] \quad (**)$$

when applied to the linear system. The same holds true for a number of modifications that have been proposed for dealing with stiff systems eg. Enright's second derivative methods (1973), the AM-BD blends of Skeel and Kong (1977) and linearly implicit methods of Sanz-Serna (1981).

Our main result is to note that when a "multistep approximation" of form (**) and order p is used for e^{hA} in (*) along with $(p-1)$ -st order interpolating polynomial for $f-Ay$ we obtain a p -th order method. In particular, the methods referred to above can be derived in this way. A

typical observation from this point of view is that the methods of Enright and those of Skeel and Kong make use of the same "multistep approximation" but differ in the choice of the interpolating polynomial.

We also briefly discuss alternative ways of dealing with varying stepsizes that suggest themselves from this new viewpoint as well as the idea of using linearly implicit and fully implicit methods as predictor-corrector pairs.

Multirate Integration Methods

Stig Skelboe, University of Copenhagen

In the simulation of many physical systems, the solution components can be separated in two or more groups with widely varying rate of change. Classical discretization methods use the same mesh for the discretization of all parts of the system while multirate methods adapt the mesh for each subsystem to the rate of change of the variables describing each particular subsystem.

Although multirate methods are conceptually simple, unsolved problems regarding their theory and implementation have inhibited practical use. This paper discusses an experimental implementation which employs a detection algorithm for the slowly varying subsystems. The detection algorithm controls the extrapolation of the slowly varying solution components to avoid recomputation of a long step (on which many short steps depend). The experimental implementation uses backward differentiation formulas based on divided differences for the change of steplength and for error estimation. Algorithms and strategies for changing the partitioning of the system are presented.

The interplay between rapidly and slowly varying subsystems has been analysed, and it has been demonstrated how a recent technique called "waveform relaxation" relates to multirate integration methods and provide a theoretical framework for an iterative integration of fast-slow-fast-etc. subsystems.

Stability Analysis of Hopscotch Methods for Fourth Order Parabolic Equations

G L G Sleijpen*, E J W Ter Maten, *University of Utrecht, The Netherlands

Often a fourth order parabolic PDE (partial differential equation) can be represented by a (system of) PDE(s) with a first order time derivative and a second order spatial differential operator that is anti-hermitian. In order to approximate the solution of these PDEs, we apply the hopscotch methods and a fast variant form, the so-called skate methods, to the ordinary differential equation that arises by a discretization of this spatial differential operator. In this way, we also find new (and known) finite difference methods for the fourth order PDEs. We discuss briefly the relations between all these methods (those for this fourth order as well as those for this PDE system). In particular we find a unified way to analyse their stability properties.

Often the error propagation of these methods can be described by a three term matrix-vector recursion in which the matrices have a certain anti-hermitian structure. We give conditions on the matrices under which this recursion is stable. These conditions are rather sharp and are fairly easy to check. In our applications to the hopscotch methods, for fixed stepsizes, we find stability results (with an error bound that is uniform

with respect to the time level) for general (autonomous) spatial differential operators (with variable coefficients and mixed derivatives).

We also derive convergence statements (i.e. when the stepsizes tend to zero).

Stability of a Boundary Condition for a Fourth Order Hyperbolic Difference Scheme

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A family of boundary conditions is considered for the solution of hyperbolic equations by means of a leap frog method which is fourth order in space and second order in time. The boundary technique is a generalisation of the uncentred scheme which has been analysed by Oliger (1974). Here we examine the accuracy and stability of the family of boundary conditions and select the optimum member of the family in terms of accuracy. Numerical experiments support the theoretical predictions.

The Existence of Solutions to the Algebraic Equations in Implicit Runge-Kutta Methods

M N Spijker, University of Leiden, The Netherlands

This paper deals with implicit Runge-Kutta methods for the numerical solution of stiff systems of, say s , (nonlinear) ordinary differential equations. We denote the number of stages of a Runge-Kutta method by m and characterize a method, as usual, by a coefficient scheme (A/b) . Here $A = (a_{ij})$ is an $m \times m$ matrix and b is a row vector with components $b_1, b_2, \dots, b_m$.

Burrage, Butcher [1] and Crouzeix [2] investigated the interesting concept of B-stability for Runge-Kutta methods. This concept is a natural extension of the notion of A-stability for non-linear differential equations. B-stability was proved to be equivalent to a simple algebraic condition on the coefficients a_{ij}, b_j (see loc. cit. and [5]). If a method fulfills this condition it is called algebraically stable.

Any algebraically stable method is necessarily implicit. Therefore, in each integration step by such a method, one arrives at a system of $m \times s$ simultaneous (nonlinear) equations. It has been conjectured for some time (and it has also been assumed tacitly in the publications mentioned above) that algebraic stability implies the existence and unicity of a solution to this system of $m \times s$ equations.

In [3] the above conjecture is shown to be false. In order that a unique solution exists the requirement of algebraic stability has to be supplemented by some further algebraic condition on the coefficients a_{ij} . Such a condition is given in [3], [4]. In the present paper we review and extend some of the results contained in [3], [4].

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Computation of Stress Intensity Factors

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We consider a two-dimensional plane stress problem of fracture mechanics, and the series expansion of the stress function around a tip of a crack. Two explicit expressions for the coefficients of this series have been found, permitting the numerical evaluation of these coefficients. Mode I has been investigated throughout and methods for dealing with more general problems is suggested.

Variational Methods for Solving Free Boundary Problems

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The role and difficulties concerning the use of trial free boundary methods for solving free boundary problems are well-known. An alternative approach, variational inequalities, has a more theoretical foundation but it can be difficult to get the problem in the right form and the accuracy achieved is not always very great.

Purely variational methods have been proposed by Betts (1) and O'Carroll (3) and an alternative approach by Varoglu and Finn (4) for solving water flow over a weir; these ideas are based on earlier work by Luke (2). Whilst having a theoretical foundation there is no analysis on these methods but they appear to work well for the problem chosen.

Here we investigate variational methods of both the Betts/O'Carroll and also the Varoglu and Finn types for solving a simple free boundary problem associated with an ordinary differential equation. Some of the difficulties and problems associated will be discussed.

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A Kantarovic Computational Method for Free Surface Gravity Flows

E F Toro*, M J O'Carroll, University of Leeds

Solutions of the non-linear problem governing potential flows with a free surface (under gravity), are stationary points of a functional $J(h(x), \psi(x, y))$. The arguments of J are a function $h(x)$ that determines the free surface position (and hence the flow domain) and the stream function ψ which gives the internal flow field.

A Kantarovic approximation reduces the full problem to a system of N non-linear ordinary differential equations in N unknown functions $h_i(x)$. These functions give the position of N streamlines, including that of the free surface. For the special case $N=1$ the model represents a type of non-linear shallow approximation for which analytical solutions in terms of cnoidal functions are obtained.

For arbitrary N , the full boundary value problem is reduced to a system of non-linear algebraic equations. These equations are efficiently solved by a Newton Raphson iteration procedure. Considerable savings in computing time and storage are made by (i) using the banded nature of the Jacobian matrix and (ii) providing the algebraic equations and the entries of the Jacobian by analytical expressions.

The algorithm is fast and stable. It is also easy to implement when solving practical problems. Applications include computing critical flows over weirs and non-linear water waves. Numerical results are in good agreement with published data (experiential and theoretical)

D-stability and Kaps-Rentrop Methods

M Van Veldhuizen, Vrije Universiteit, Amsterdam

A Kaps-Rentrop method is not D-stable. In practice this lack of D-stability may show up in at least two ways: an excessive number of steps is required and/or the error in the results is very large. By means of a simple model we are able to define two quantities. The value of these quantities is an indicator for the kind of behavior of a Kaps-Rentrop method in instances where the lack of D-stability is felt. These quantities, functions of the coefficients of the method, will be described. Optimal Kaps-Rentrop methods of order four will be given, as well as illustrative numerical results.

The Structure of the Moving Finite Element

A J Wathen*, M J Baines, University of Reading

The Moving Finite Element Method for evolutionary partial differential equations leads to a coupled non-linear system of ordinary differential equations in time, with a coefficient matrix A , say. We show that, for linear elements in any number of dimensions, A can be written in the form $M^T C M$ where the matrix C depends solely on the mesh geometry and the matrix M on the gradient of the solution. As a simple consequence we show that A is singular only in the cases (i) element degeneracy ($|C| = 0$) and (ii) collinearity of nodes (M not of full rank). We give constructions for the "inversion" of A in all cases.

In one dimension if A is non-singular, it has a simple explicit inverse. If A is singular we replace it by a reduced matrix A' . We show that in every case the spectral radius of the Jacobi iteration matrix is $1/2$.

Finally, we discuss the applicability of these arguments to systems of equations in any number of dimensions.

Computation of Symmetry-Breaking Bifurcation Points

Bodo Werner*, Alastair Spence, University of Hamburg

Bifurcation points of parameter dependent nonlinear equations $g(\lambda, x) = 0$ (e.g. turning points, simple bifurcation points, cusp points,...) can be often characterized as isolated solutions of certain "extended systems of

nonlinear equations". This can be used for their numerical computation. (Seydel (1979), Moore/Spence (1980), Moore (1980), Spence/Werner (1982), Weber (1980)). In this talk "symmetry breaking bifurcation points" (pitchfork bifurcation points or double turning points) are treated for problems with an underlying symmetry condition

$$g(\lambda, Sx) = Sg(\lambda, x), \quad S \neq \text{Id.}, \quad S^2 = \text{Id.}$$

It can be shown that those points are isolated solutions of rather simple extended systems of equations. Numerical examples are given.

The Stability and Accuracy of Semi-discretised Schemes in the Numerical Solution of Hyperbolic Differential Equations

R A Williamson, University of Cambridge

Using the theory of order stars the relationship between the accuracy and stability of semi-discretised finite difference schemes for the advection equation $u_t = u_x$ is investigated. Given the scheme

$$\sum_{j=-R}^S f_j \frac{d}{dt} u_{k+j}^n = \sum_{j=-r}^s g_j u_{k+j}^n$$

of accuracy p it is established that, subject to stability, $p < \min [r+s+R+S, 2(r+R+1), 2(s+S)]$. Furthermore, using Pade theory, stable methods which attain this bound on accuracy for various choices of r, s, R and S are obtained.

Local Convergence in Inexact Newton Methods

T J Ypma, University of the Witwatersrand, South Africa

We provide a simple, affine invariant condition which ensures local convergence of inexact Newton methods. This condition is used to establish the convergence of Newton-like methods in which the iteration is perturbed by rounding errors.

An Example of Only Linear Convergence of Trust Region Algorithms for Nonsmooth Optimization

Y Yuan, University of Cambridge

Most superlinear convergence results about trust region algorithms for nonsmooth optimization are dependent on the inactivity of trust region restrictions. An example is constructed to show that it is possible that at every iteration the trust region bound may be active and the rate of convergence is only linear, though strict complementarity and second order sufficiency conditions are satisfied.

Two-parameter family of linearly implicit methods which avoid the exactness of the Jacobian for solving stiff ODEs

H Zedan, University of Bristol

A class of Rosenbrock-type methods for solving stiff systems of ordinary differential equations is presented. These methods allow the use of the inexact Jacobian matrix of the system during the integration. A second order two-parameter family of such methods with built-in error estimate is constructed. A particular case of this family is taken and tested over a variety of stiff systems. The test shows the efficiency and comparability

of the method over some existing ones.

On Search Times of Direction Set Algorithms

You Zhaoyong; Chengxian Xu, Xi'an Jiaotong University, China

If f on R^n is not differentiable, the direction set algorithm suggested by Powell which is used to determine the minimal point x^* of f on R^n is effective. Recently, much work has been done to improve the algorithm because of the n^2 line searches used by the method and the linear dependence of the search directions which can easily take place.

In this paper, the result that the line search times needed in this kind of algorithm is $n(n+1)/2$ in the general case is proved and a new direction set algorithm suggested.

Theorem 1. The minimal points of quadratic positive function $Q(x)$ on $(n-k+1)$ parallel k -dimensional planes π_k^i , $i = 1, \dots, n-k+1$ form a $(n-k)$ dimensional plane S_{n-k} which is A -conjugate with π_k^1 and the minimal point x^* of Q is on S_{n-k} .

Theorem 2. Let $Q(x) = x^T A x + b^T x + c$, A is a symmetric positive matrix, Then there are n A -conjugate directions in R^n and the minimal point x^* of Q can be obtained by carrying out $n(n+1)/2$ accurate line searches.

The steps of the new direction set algorithm, which is called the decreasing dimension method, are as follows:

1. Given the first point x_1 and directions $p_i = e_i$, $i = 1, 2, \dots, n$, let $k := j$ and $p_1^k := p_1$.
2. $x_j = x_1 + \epsilon p_j$, $j = 1, 2, \dots, n$, $\epsilon \neq 0$.
3. Line searches. $f(x_j + \lambda_j p_j) = \min_{\lambda} f(x_j + \lambda p_j)$, $x_{n+j} = x_j + \lambda_j p_j$, $j = 1, 2, \dots, n$.
4. To construct orthogonal directions.

$$\bar{p}_{j-1} = x_{n+j} - x_{n+1}, \quad j = 2, \dots, n, \quad k := k+1, \quad p_1^k = \bar{p}_1$$

$$p_j := \bar{p}_j - \sum_{r=1}^{j-1} \frac{(\bar{p}_j, p_r)}{\|p_r\|^2} p_r, \quad j = 2, \dots, n-1.$$

5. Let $n := n+1$, $x_1 := x_{n+1}$, goto step 2.

The convergence rate of this algorithm is proved to be quadratic, that is,

Theorem 3. The direction sequences (p_1^k) $k = 1, 2, \dots, n$ which are generated from the algorithm for the function Q are A -conjugate.

Global Iteration Methods for Strongly Monotone Operator Equation and Application to Finite Element Solution of Nonlinear Problem

You Zhaoyong; Xu Zongben, Xi'an Jiaotong University, China

In this article we introduce the definitions of a operator that is upper controlled by a functional as well as has continuity of an upper-controlled function. Under the assumption that operator A respectively coincides with the definitions, we establish a class of

global iteration methods for strongly monotone operator equation $Ax=b$, which extend all of the results obtained by Bruck [1], Dotson [2], Nevanlinna [4] and You Zhaoyong [3]. As an application, for a class of nonlinear elliptic boundary value problems, it is shown that the finite element solution of this class of problems can be generated by using iteration methods rather than solving nonlinear simultaneous equations. Especially, the iteration only requires evaluation of integrals, so that it's practical use is very convenient.

Selfadaptive Time-integration in a Code for Numerical Treatment of an Air Pollution Model

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The long-range transport of airpollutants over Europe is modelled by a system of advection-diffusion partial differential equations (PDE's). Package ADM (Advection-Diffusion Modelling) is used in the numerical solution of the system of PDE's. A pseudospectral (Fourier) algorithm is applied in the discretization of the first-order space derivatives [5]. The stability restrictions caused by the second-order space derivatives are removed by the use of a special device for discretization of these derivatives [6]. A large system of ordinary differential equations (ODE's) is obtained after the space discretization. Several different algorithms for solving ODE's can be specified. An option, where the time-integration part of the solution of the system of PDE's is fully automatized, is available. A variable stepsize variable formula method, VSVFM, based on time-integration algorithms proposed and/or studied in [1-4,7,8], is built-in in this option. The efficiency of the VSVFM option in package ADM is demonstrated by numerical examples in which real meteorological data prepared within project EMEP (European Monitoring and Evaluation Program) are applied. Project EMEP is a common European project in which practically all European countries participate. Comparisons of the calculated concentrations of sulphur di-oxide and sulphate with observations at different stations in the countries which participate in project EMEP is presented.

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