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Abstracts

Section A: Invited Talks

Section B: Submitted Talks

Section A: Invited Talks

FINITE ELEMENT APPROXIMATION OF DEGENERATE QUASILINEAR ELLIPTIC AND PARABOLIC PROBLEMS

John W. Barrett (Imperial College) & **Wenbin Liu** (Imperial College).

In this talk we prove energy type error bounds for the finite element approximation of the following quasilinear elliptic problem:

Given $k \in C(0, \infty)$ satisfying $k(s), [k(s)s]' \geq 0 \quad \forall s \geq 0$ and f, g ; find u s.t.

$$-\nabla \cdot (k(|\nabla u|) \nabla u) = f \quad \text{in } \Omega \subset \mathbb{R}^2, \quad u = g \quad \text{on } \partial\Omega.$$

The above problem is degenerate if $k(0) = 0$ or ∞ ; e.g. the p -Laplacian, when $k(s) \equiv s^{p-2}$ for a given $p \in (1, 2) \cup (2, \infty)$. These error bounds improve on existing results in the literature and are often optimal for sufficiently regular solutions, which we show to be achievable for a subclass of data f, g and Ω . A key step in the analysis is to prove abstract error bounds initially in a quasi-norm, which naturally arises in degenerate problems of this type.

We extend these results to the corresponding parabolic case and to the corresponding obstacle problems (variational inequalities). Finally, we extend these results to the non-Newtonian flow problem:

Given $k(\cdot)$ as above and f ; find a velocity $\underline{u}$ and a pressure q s.t.

$$\begin{aligned} -\sum_{j=1}^2 \frac{\partial}{\partial x_j} [k(|D(\underline{u})|) D_{ij}(\underline{u})] + \frac{\partial q}{\partial x_i} &= f_i \quad \text{in } \Omega \subset \mathbb{R}^2 \quad i = 1, 2, \\ \nabla \cdot \underline{u} &= 0 \quad \text{in } \Omega, \quad \underline{u} = \underline{0} \quad \text{on } \partial\Omega, \quad \int_{\Omega} q = 0; \end{aligned}$$

where $D(\underline{u})$ is the rate of deformation tensor, i.e. $D_{ij}(\underline{u}) \equiv \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ $i, j = 1, 2$; and $|D(\underline{u})|^2 \equiv D(\underline{u}) \cdot D(\underline{u}) \equiv \sum_{i,j=1}^2 |D_{ij}(\underline{u})|^2$.

THE SOLUTION OF AUGMENTED SYSTEMS

Iain S Duff (Rutherford Appleton Laboratory, CERFACS, and University of Strathclyde)

We examine the solution of sets of linear equations for which the coefficient matrix has the form

$$\begin{bmatrix} H & A \\ A^T & 0 \end{bmatrix}$$

where the matrix H is symmetric.

These augmented systems are ubiquitous arising, for example, in the solution of linear programming problems, constrained optimization, differential algebraic systems, and computational fluid dynamics.

We are interested in the case when the matrices H and A are sparse and concentrate on direct methods of solution. We examine issues related to conditioning and scaling, and discuss the design and performance of a code for solving these systems.

NUMERICAL SOLUTION OF THE PHASE FIELD EQUATIONS

C M Elliott (University of Sussex)

The phase field equations arise in the modelling of the solidification of undercooled liquids.

They are the coupled parabolic equations:-

$$c\theta_t + \frac{1}{2}u_t = k\Delta\theta$$

$$\tau u_t = \gamma \Delta u - \psi'(u) + \alpha \theta$$

where ψ is a double well potential, say $\psi(u) = \frac{1}{4}(u^2 - 1)^2$. By choosing an appropriate scaling of τ , γ and α with respect to a small parameter ϵ the phase field equations are a regularisation of a moving boundary problem for the heat equation $c\partial_t = k\Delta\theta$. In this talk we discuss the numerical issues which arise in the use of the phase field equations to compute curvature dependent boundary motion.

SOLVING REDUCED KKT SYSTEMS IN BARRIER METHODS FOR LINEAR AND QUADRATIC PROGRAMMING

Philip E. Gill (University of California, San Diego)

In barrier methods for constrained optimization, the main work lies in solving large linear systems $Kp = r$, where K is a symmetric and specially structured indefinite matrix.

For linear programs, these KKT systems are usually reduced to smaller positive-definite systems $AH^{-1}A^Tq = s$, where H is a large principal submatrix of K . These systems can be solved more efficiently, but $AH^{-1}A^T$ is typically more ill-conditioned than K .

We discuss the theoretical and practical aspects of two recent approaches that give reduced KKT systems other than $AH^{-1}A^T$. The first, proposed by Vanderbei, is intended to provide a system that can be factorized with only 1×1 pivots and no row or column interchanges. The second is designed to give a reduced system whose dimension and condition lie somewhere in between those of K and $AH^{-1}A^T$.

THE DYNAMICS OF A DISCRETISED NONLINEAR DELAY DIFFERENTIAL EQUATION

Desmond J. Higham (University of Dundee)

We consider a delay-logistic differential equation that has important applications in population dynamics. We set up a constant-stepsize discretisation of the problem and examine the long term behaviour of the solution. Key differences between this problem and the more familiar non-delay version are that

- (i) introducing a small delay improves the stability of the iteration
- (ii) for a certain parameter range, the stable steady state loses stability through a complex eigenvalue, and
- (iii) spurious solutions exist even when the stepsize is stable in a linear sense.

We also consider a variable-stepsize version of the discrete method, based on a standard local error estimate. Tests reveal that the error control suppresses spurious behaviour, and we give some theoretical arguments to support these observations.

DIFFERENTIAL-ALGEBRAIC EQUATIONS AND CONTROL SYSTEM DESIGN

N.K. Nichols (University of Reading)

Control systems governed by implicit differential-algebraic equations arise in a variety of practical contexts, including aircraft guidance, chemical processing, mechanical body motion, power generation and others. The response of these systems, called 'descriptor' or 'generalized state-space' systems, can have a complicated structure and may even contain impulsive modes. Numerical methods are needed to assess the properties of these systems and to aid system design. The main computational tool used for both system analysis and design synthesis is the reduction of the system by unitary transformations to a condensed matrix form. Such forms reveal both the structure of the system and the degrees of freedom available for the design. The synthesis problems are generally under-determined, and it is desirable to select the free parameters to obtain 'robust' designs that are insensitive to plant disturbances and model uncertainties.

In this paper we examine two computational techniques for achieving robust designs - eigenstructure assignment and singular value assignment. These methods are used in solving two basic synthesis problems: the design of automatic controllers by proportional and derivative feedback and the design of observers (or state-estimators) for estimating the states of a system from measured data. Applications to various practical cases are presented, including gas flow estimation and aircraft guidance.

AN ITERATIVE METHOD FOR THIN PLATE SPLINE INTERPOLATION

M J D Powell (University of Cambridge) & *R.K. Beatson* (University of Canterbury, New Zealand).

Thin plate spline interpolation to functions of two variables is useful in many applications, because there are few restrictions on the positions of the data points. Further, some smoothness properties are achieved naturally, because the interpolant minimizes a second derivative norm subject to the interpolation conditions. On the other hand, full matrices occur and there may be several thousand data points. Therefore we ask whether adequate approximations to the Lagrange functions of the interpolation calculation can be constructed from small subsets of the data points. We find that the smoothness and decay properties of thin plate splines allow the construction of such estimates. The coefficients of these estimates provide a sparse approximation to the inverse of the interpolation matrix, which we use in a simple iterative refinement procedure. Thus we develop a method for thin plate spline interpolation that may be highly efficient when the number of data points is large. The work was incomplete, however, when this abstract was written.

ERRING AND BEING CONSERVATIVE

J.M. Sanz-Serna (University of Valladolid, Spain) & *J. de Frutos* (University of Valladolid, Spain).

When numerically integrating time-dependent differential equations, it is often recommended to employ methods that preserve some of the invariants (mass, energy, etc.) of the problem being considered. This recommendation is usually justified on the grounds that conservation of invariant quantities may ensure that the numerical solution possesses some important qualitative features. However there are cases where schemes that preserve invariants are also advantageous in that they possess favourable error propagation mechanisms that render them superior from a quantitative point of view. In the talk we consider the Korteweg-de Vries equation as a case study. Perturbation theory results are presented along with functional analysis material and numerical experiments.

ON THE ERROR DUE TO THE STOPPING OF THE NEWTON ITERATION IN IMPLICIT LINEAR MULTISTEP METHODS

M. N. Spijker (University of Leiden, the Netherlands)

This paper concerns the numerical solution of initial value problems for nonlinear ordinary differential equations by implicit linear multistep methods.

For non-stiff problems, fixed point iteration (Picard iteration), is a classical approach to the solution of the system of algebraic equations occurring in each step of these methods. The order of the error due to the stopping of this process after a fixed number of iterations is well understood.

For stiff problems, Picard iteration is not appropriate and some variant of the Newton method is usually used instead. This paper addresses the problem of estimating the

stopping error of Newton-like iterations. We aim for an understanding of this error comparable to what is known about Picard iterations. Because of stiffness, the theory is more delicate than for Picard iterations.

UTV DECOMPOSITIONS

G. W. Stewart (University of Maryland)

People who work with nearly rank degenerate matrices have traditionally used one of two decompositions. The first is the singular value decomposition in which the matrix A is factored in the form $A = UDV^T$, where U and V are orthogonal and D is diagonal. The near degeneracy of A exhibits itself in small diagonal elements. The alternative is the pivoted QR decomposition, in which A is factored in the form $A = QRP$, where Q is orthogonal, R is upper triangular, and P is a permutation matrix. The degeneracy shows up as a small trailing principal submatrix.

Recently, a new class of orthogonal-triangular-orthogonal decompositions have been proposed. Here A is factored in the form $A = UTV^T$, where U and V are orthogonal and T is triangular. Degeneracy shows itself in near zero columns or rows of T . These decompositions are computationally less expensive than the singular value decomposition and more flexible than the pivoted QR decomposition. In this talk we will give a survey of these UTV decompositions.

APPROXIMATION THEORY FOR ATTRACTIVE INVARIANT MANIFOLDS

Andrew Stuart (Stanford University)

Attractive invariant manifolds for evolution equations are fundamental in understanding long time dynamics. The purpose of this work is to study the behaviour of such manifolds under approximation.

The abstract evolution equation

$$u_t + Au = F(u), \quad u(0) = u_0$$

is considered. Using spectral projections associated with the linear operator A , the solution $u(t)$ is split into a finite dimensional part $p(t)$ and its complement $q(t)$. Thus $u(t) = p(t) + q(t)$ and the equation may be written as a pair of coupled equations in the form

$$\begin{aligned} p_t + Ap &= PF(u), & p(0) &= Pu_0 \\ q_t + Aq &= \{I - P\}F(u), & q(0) &= \{I - P\}u_0. \end{aligned}$$

Assumptions on A and F are made sufficient for the existence of an attractive invariant manifold of the form $q = \Phi(p)$.

A general approximation theory is formulated using semigroups; using this theory it is shown that standard approximations, encompassing finite difference, finite element, spectral and time discretisation, have an approximate attractive invariant manifold Φ^ϵ which converges to Φ as the approximation is refined.

Applications are described in the context of both inertial manifolds and unstable manifolds. Equations considered include a reaction-diffusion problem, the Navier-Stokes equation and the Kuramoto Sivashinsky equation. The approximation results are employed to make deductions about the structure of the attractor and the flow on the attractor under discretisation.

This is joint work with Don Jones, Center for Turbulence Research, Stanford University.

A LOWER BOUND ON THE NUMBER OF ITERATIONS OF AN INTERIOR-POINT ALGORITHM FOR LINEAR PROGRAMMING

M J Todd (Cornell University, USA)

We describe some elements of interior-point methods for linear programming problems. In contrast to Dantzig's well-known simplex method, these algorithms generate a sequence of points in the relative interior of the feasible region. They have remarkable properties: some of these methods have attractive theoretical bounds on the number of iterations, while others can be highly effective – recently a problem with more than 12 million variables was solved in a few minutes on a Cray Y-MP. We discuss a particular algorithm (the primal-dual affine-scaling method) very close to those implemented in practice, and demonstrate that it may take a number of iterations growing with the cube root of the number of variables. In so doing, we will solve "by hand" (or at least take a couple of iterations for) a 2 million variable problem.

COMPUTATIONAL ANALYSIS IN RHEOLOGICAL FLUID DYNAMICS

P. Townsend (University of Swansea)

Numerical techniques have been well established as essential tools in the study of classical fluid dynamics for quite some time. For the study of the flow of rheologically complex fluids the picture is rather different. It is only relatively recently that one has seen the emergence of commercially available software packages specifically designed for this area. Even these have their limitations and there are many unresolved problems to tax the abilities of the numerical analyst. In this talk a brief survey will be given of some of these problems in the context of particular applications in the process industry. A finite element technique, which may be used to address such problems, will be described, and some results presented to illustrate the effectiveness of the technique.

Section B: Submitted Talks

REDUCING THE DEGREE OF BÉZIER CURVES

M.L. Baart (Potchefstroom University for C.H.E., South Africa) & M.A. Coetzee (Potchefstroom University for C.H.E., South Africa).

Various methods for reducing the degree of Bézier curves have been introduced, for example by Watkins and Worsey in 1988. We found that all of these methods lead to discontinuity if you want to reduce the degree of curves consisting of two or more segments of coplanar cubic Bézier curves. Watkins and Worsey suggested that this problem can be eliminated by keeping the endpoints of the segments fixed. This guarantees C^0 continuity, but it is more difficult to retain C^1 (or more specifically G^1) continuity. We suggest two methods for solving this problem, and discuss the generalization of these methods to curves of higher degree.

1. Farin, G., *Curves and surfaces for computer-aided geometric design*, Academic Press, 1988.
2. Gregory, J.A., Geometric Continuity, in *Mathematical Methods in CAD*, Academic Press, 1989, 353–371.
3. Watkins, M.A. and Worsey, A.J., Degree reduction of Bézier curves, *Computer-Aided Design*, 1988, 398–405.

ADAPTIVE GRID GENERATION AND MONOTONIC ADAPTIVE SOLUTIONS OF TIME DEPENDENT PDE'S

M. J. Baines (University of Reading)

A direct minimisation of the L_2 error between a continuous function and its approximation using discontinuous linears with variable nodes can be used to generate data-dependent grids for which the mesh never tangles.

A moving grid algorithm for time-dependent PDE's is described based on this idea in which a local recovery plays a part.

ON THE STABILITY OF LINEAR MULTISTEP FORMULAE ADAPTED FOR VOLTERRA FUNCTIONAL EQUATIONS

Christopher T H Baker (University of Manchester)

Linear multistep formulae for ordinary differential equations can be adapted for numerical solution of Volterra functional equations such as delay-differential equations and integro-differential equations. We present a unified theory for stability analysis of constant-coefficient recurrence relations arising when such formulae are applied to linear test equations. In particular, it is noted that the (strict) stability of the adapted formulae applied to basic delay-differential equations and integro-differential equations that are parameterized by ξ, η , and using a step $h > 0$, is governed by the requirement that some corresponding function $\hat{S}_h(\xi, \eta; \zeta)$ does *not* vanish for $|\zeta| \leq 1$. There follow, from this, sets of sufficient conditions for stability, in terms of some functions ι_1 and ι_2 defined solely by the underlying LMF. We emphasize the unifying aspect of our discussion.

THE STRUCTURED TOTAL LEAST SQUARES PROBLEM

Sven G. Bartels (Universität Karlsruhe, Germany)

The classical total least squares technique for solving overdetermined systems of linear equations does not account for structure in the coefficient matrix. We introduce an extension such that the perturbed matrices keep their structure. The case of Toeplitz

and of Vandermonde matrices are discussed in detail and illustrated through numerical examples

ORTHOGONALITY-PRESERVING DIFFERENCE EQUATIONS AND AN APPLICATION TO THE ANALYTIC SINGULAR VALUE DECOMPOSITION

S. Bell (University of Reading)

A method for approximating matrix equations of the form $X' = W(X, t)X$ where W is skew-symmetrical and X is orthogonal is presented. Standard difference schemes do not give an orthogonal approximation to the solution of such an equation—loss of orthogonality is of the same order as the global error. The method given, however, preserves orthogonality to machine precision.

This method is then applied to finding an Analytic Singular Value Decomposition (ASVD) of a matrix $E(t)$. This is a time varying decomposition path of a matrix whose elements are analytic functions of t . It is shown that the problem of finding an ASVD can be reduced to solving a set of three systems of linear equations, two of which are of the above form. A cheap and accurate algorithm for calculating the ASVD is given, along with test examples.

A FINITE ELEMENT ESTIMATE WITH TRIGONOMETRIC HAT FUNCTIONS FOR STURM-LIOUVILLE EIGENVALUES

G. Vanden Berghe (University of Gent) & H. De Meyer (University of Gent).

In the last few years, there has been much interest in numerical methods requiring efficient and accurate computation of a long sequence of eigenvalues of regular Sturm-Liouville problems. Andrew and Paine have shown, in several papers, that the error on the eigenvalues for zero potential functions has the same asymptotic form for a high-lying eigenvalue as the error for a general potential function. The present authors have used previously a step-dependent linear multistep method and a modified Numerov method and have shown that the eigenvalues derived in that way, were as accurate as the asymptotically corrected ones of Andrew and co-workers. In this contribution it is shown that the error of a high-lying eigenvalue obtained by a finite element method with trigonometric hat functions and mesh length h is of the same order as the one obtained with classical linear functions together with a simple asymptotic correction technique of Andrew et al.

LEBESGUE CONSTANT MINIMIZING LINEAR RATIONAL INTERPOLATION OF CONTINUOUS FUNCTIONS OVER THE INTERVAL

Jean-Paul Berrut (Université de Fribourg, Switzerland)

As printed in every numerical analysis book, polynomial interpolation between large numbers of arbitrary nodes does not in general yield useful approximations of continuous functions. Good results can only be expected for regularly distributed nodes (on the circle), whose Lebesgue constant Λ is small. This fact is usually explained by looking at polynomial interpolation as a linear projection whose norm equals Λ : the interpolation error is at most $(1 + \Lambda)$ times the error of the best approximation by any polynomial of the same degree. It is then natural to consider as optimal for polynomial interpolation those nodes for which Λ is smallest.

In order to find a good interpolant for arbitrary nodes, we first notice that polynomial interpolation of a fixed degree, say n , can be seen as linear rational interpolation whose denominator is a constant, thus independent of the interpolated function and of the nodes. We suggest here to determine for each set of $n + 1$ nodes another denominator of

degree n and to interpolate every continuous functions by a rational function with that same denominator, so that the resulting interpolation process remains a linear projection. Our optimal denominator is chosen so as to minimize the Lebesgue constant for the given nodes. It (probably) has to be computed numerically. For that purpose, we use the barycentric representation of rational interpolants, which displays the linearity of the interpolation and reduces the determination of the denominator to that of the barycentric weights. The optimal weights for given nodes can then be computed by solving with respect to the weights an optimization problem with simple bounds. And in a next step the optimal nodes can be found as those minimizing that weight optimal Lebesgue constant.

THE NUMERICAL ANALYSIS OF A MODEL FOR PHASE SEPARATION OF A MULTI-COMPONENT MIXTURE

J.F. Blowey (University of Durham) *M.I.M. Copetti* (University of Santa Maria, Brazil) & *C.M. Elliott* (University of Sussex).

We consider the numerical analysis of a model for multi-component phase separation suggested by Elliott & Luckhaus [1991]. It is a system of nonlinear diffusion equations, modelling isothermal phase separation of an ideal mixture of $N \geq 2$ components occupying an isolated domain. In particular, when $N = 2$ these equations correspond to the Cahn-Hilliard equation with logarithmic free energy. Some interesting numerical simulations will also be presented.

DISCRETE LEAST SQUARES APPROXIMATION AND PREWAVELETS FROM RADIAL FUNCTION SPACES

M.D. Buhmann (University of Cambridge)

In this talk we shall study convergence behaviour of least squares approximations of various types by radial basis functions, i.e. least squares approximations from spaces spanned by radially symmetric functions $\phi(\|\cdot - x_j\|)$. Here the x_j are given "centres" in $\mathcal{R}^n$ which we assume to lie on a grid. The inner products with respect to which the least squares problem is considered are discrete and Sobolev, i.e. may involve derivative information. Favourable estimates for the least squares errors are found that are shown to decrease as powers of the gridspacing. The work on discrete least squares approximations also gives rise to the construction of *prewavelets* from radial function spaces with respect to a discrete Sobolev inner product, which are discussed in the talk as well.

THE HEAT BALANCE INTEGRAL METHOD FOR CYLINDRICAL AND SPHERICAL PROBLEMS

J. Caldwell (City Polytechnic of Hong Kong)

In this paper we study the numerical solution of melting/solidification problems using the Heat Balance Integral Method (HBIM). This method first propounded by Goodman and later extended by Bell is applied to model problems arising from the partial differential diffusion equation. Bell's method substantially increases the accuracy of solution by sub-division of the region. The HBIM is applied to both a cylindrical and spherical problem. Both problems suffer the complication of having a singularity at $t = 0$ in the resulting system of ODE's for which a special starting procedure is required. The accuracy achieved even with a limited sub-division using a linear profile compares favourably with that obtained from other more complicated methods. The numerical results obtained are discussed and conclusions are drawn.

SOME RECENT RESULTS ON SYMPLECTIC INTEGRATION

M. P. Calvo (Universidad de Valladolid, Spain)

B-series provide a powerful tool to express numerical methods for differential equations. Many differential equations are of Hamiltonian form and then it makes sense to ask under which conditions a B-series corresponds to a canonical method. In the talk, necessary and sufficient conditions are given for a B-series to be canonical. On the other hand, numerical results are presented for the Morse oscillator problem, comparing symplectic and nonsymplectic Runge-Kutta-Nystrom methods.

THE FINITE SECTION METHOD FOR INTEGRAL EQUATIONS ON THE HALF-LINE IN WEIGHTED SPACES

Simon N Chandler-Wilde (University of Bradford)

The first stage in most approximate solution methods for integral equations on the half-line, particularly those of Wiener-Hopf and related type, is the replacement of the full half-line integral operator by one for which the integration is restricted to the finite interval $[0, b]$, for some $b > 0$. The locally uniform convergence of the corresponding "finite section approximation" to the solution of the original integral equation as b tends to infinity was proved in Anselone and Sloan (1985) for a subset of equations on the half-line including those of Wiener-Hopf type.

Frequently, it is not uniform convergence which is of interest but convergence in a weighted space, where more weight is given to errors at points far from the origin. Under natural assumptions on the decay with distance from the diagonal $s = t$ of the kernel $k(s, t)$ of the half-line integral operator, we prove that the finite section method is stable in certain weighted spaces of continuous functions if it is stable in the space of bounded continuous functions on the half-line. As a particular application we apply our results to a class of integral operators which includes all compact perturbations of Wiener-Hopf operators and certain non-compact perturbations as well.

QUALITY ASSESSMENT OF ADAPTIVE QUADRILATERAL MESHES BY FUNCTION INTERPOLATIONS

Ke Chen (University of Liverpool)

The generation of adaptive grids which can capture the main features of the underlying data (or solutions in solving operator equations) is of great importance. In this talk, we first discuss various strategies of generating adaptive data dependent quadrilateral grids. Among them is a new strategy based on curve-by-curve equidistributions. Most of these grid systems result from minimising some interested quantities and are expressed in the form of partial differential equations (PDE's). The solution of such PDE's defines the required grid.

To assess the quality of any such grids, we would need to use them in some other contexts and observe the effects. Methods of interpolation at grid points are considered to differentiate between good and bad mesh strategies by some error criteria. Piecewise linear interpolations are tested versus some radial basis function interpolations. Some recent results will be reported.

LIMIT LOADS COMPUTED AS THE MINIMUM OF A SUM OF NORMS

Edmund Christiansen (Odense University, Denmark)

We consider the problem of finding the limit load multiplier for a given load distribution on a rigid plastic continuum, obeying the Mises yield condition. Using a mixed finite

element method the discrete problem can be formulated as a minimum problem for a sum of Euclidean norms subject to one linear constraint. In general it is necessary to use divergence free elements for the plastic flow in order to ensure that the objective function is finite.

Such a sum of norms is not differentiable, but still efficient solution methods exist. We present results in plane strain and for plates, which are considerably more accurate than previous results.

THE FABER POLYNOMIALS FOR ANNULAR SECTORS

J.P. Coleman (University of Durham) & **N.J. Myers** (University of Durham).

Applications to iterative methods in numerical linear algebra (for example, [2] and [4]) require a knowledge of the Faber polynomials for a suitable region containing relevant eigenvalues of the matrix of interest, but Faber polynomials are known explicitly only for a few types of domain. Professor G. Opfer suggested to one of the authors, during the conference dinner at the 1991 Dundee Conference, that an annular sector would be a useful general-purpose region which, by scaling and rotation, could be adjusted to enclose an eigenvalue cluster bounded away from the origin.

This paper builds on the work of Coleman and Smith [1] and of Gatermann et al [3], to provide explicit formulae for Faber polynomials for a sector of an annulus. We have constructed the function ψ which maps the complement of the unit disc $\{w : |w| \leq 1\}$ conformally onto the complement of an annular sector Q , such that

$$\psi(\infty) = \infty, \quad \lim_{w \rightarrow \infty} \frac{\psi(w)}{w} = \rho,$$

where ρ is the transfinite diameter of the domain Q . The mapping function and the transfinite diameter depend on two parameters, a and b , which are determined, in terms of the half angle of the annular sector and the ratio of its radii, by a pair of non-linear equations. The coefficients of the Laurent expansion of ψ about ∞ may be generated recursively, and then used in a recurrence relation to generate the Faber polynomials $F_n(z)$. It is possible to formulate the computation so as to allow an algebraic manipulation package to generate the coefficients of the scaled Faber polynomials $\tilde{F}_n(z) = F_n(z)\rho^{-n}$ explicitly as functions of the parameters a and b . We have used this to determine the scaled Faber polynomials of degree ≤ 15 .

Known results for an interval, a circular arc and a circular sector are obtained as special cases.

1. J.P. Coleman and R.A. Smith (1987), *The Faber Polynomials for circular sectors*, Math. Comp. 49, 231-241.
2. M. Eiermann (1989), *On semiiterative methods generated by Faber polynomials*, Numer. Math 56, 139-156.
3. K. Gatermann, C. Hoffmann and G. Opfer (1992), *Explicit Faber polynomials on circular sectors*, Math. Comp. 58, 241-253.
4. G. Starke and R.S. Varga (1993), *A hybrid Arnoldi-Faber iterative method for non-symmetric systems of linear equations*, Numer. Math. 64, 213-240.

AN ADAPTIVE SCHEME FOR THE DERIVATION OF HARMONIC IMPEDANCE CONTOURS

I. D. Coope (University of Canterbury, New Zealand) *M. Dominguez* (University of Cantabria, Spain) *J. Arrillaga* (University of Canterbury, New Zealand) & *N.R. Watson* (University of Canterbury, New Zealand).

The aim of this paper is to make the calculation of harmonic impedances accurate and efficient. An adaptive scheme is proposed which significantly reduces the number of frequency samples to be used in the derivation of the impedance/frequency loci. The scheme is then used to derive three-phase harmonic impedance contours which take into account any specified range of fundamental frequency variation.

A ONE-DIMENSIONAL QUASI-STATIC CONTACT PROBLEM IN LINEAR THERMOELASTICITY

M. I. M. Copetti (Universidade Federale de Santa Maria, Brazil) & *C.M.Elliott* (University of Sussex).

The existence, uniqueness and regularity of the solution to a one-dimensional linear thermoelastic problem with unilateral contact of the Signorini type are discussed. A finite element approximation is described and some numerical experiments are presented.

DISCRETISATION AND MULTIGRID SOLUTION OF ELLIPTIC EQUATIONS WITH STRONGLY DISCONTINUOUS COEFFICIENTS

P. I. Crumpton (Oxford University) *G. J. Shaw* & *A. F. Ware* (Oxford University & NAG ltd)

This paper introduces a new conservative cell centred finite volume scheme for accurate solution of elliptic diffusion equations with strongly varying coefficients. The discretisation is designed to model a wide range of heterogeneities and anisotropies, and in particular the case where the diffusivity is represented by a non-diagonal matrix, which may occur if the medium is anisotropic in a general direction. Such problems arise for example in oil reservoir simulation, when renormalisation techniques are used to model the reservoir geology. It is in this context that the method is described, although it is applicable to a far wider class of problems in heat conduction, electrostatics and potential theory.

The paper also describes the application of a multigrid scheme for efficient numerical solution of the algebraic equations derived using the new discretisation.

CONTINUATION AND THE DETECTION OF BIFURCATIONS IN LARGE SYSTEMS OF DIFFERENTIAL ALGEBRAIC EQUATIONS USING THE RECURSIVE PROJECTION METHOD

Bryan D. Davidson (University of Bristol)

Large parameter dependent nonlinear systems of semi-explicit differential algebraic equations (DAE's)

$$B\dot{x} = F(x, \lambda)$$

where B is singular, occur in many applications (eg. fluid dynamics, electronics, optimal control, physical chemistry, dynamic simulation of mechanical problems). Schroff and Keller (*Siam J. Num. Anal.*, June 1993) have recently developed a new algorithm (the Recursive Projection Method or RPM) which can compute stable and unstable steady states of large parametrised dynamical systems (at which B is nonsingular) by using a supported Picard continuation method. We show how the RPM can easily be adapted to compute steady states when B is singular, provided the system of DAE's is consistent and has index 1.

A key feature of our algorithm is that it tracks a path on the constraint manifold of the DAE. We show that this allows the algorithm to continue a branch of steady states, while at the same time, identifying the presence of any steady state or Hopf bifurcations on the computed path. This is done simply and efficiently without increasing the dimension of the system. Existing continuation methods cannot detect Hopf bifurcations without introducing additional variables into the problem. Thus the method offers a new approach to numerically determining steady states and linear stability in large systems of index 1 DAE's.

The advantages and disadvantages of this method and the results of some preliminary testing on some simple examples will be discussed.

ACCURATE & STABLE NUMERICAL SCHEMES FOR SCATTERING PROBLEMS

Penny J. Davies (University of Dundee) & *Dugald B. Duncan* (Heriot-Watt University).

Time marching algorithms are often used to compute the current induced on a perfect conductor by a pulsed electric field. They involve solving a coupled system of discretised PDEs and retarded potential integral equations (RPIEs). Whilst there are many excellent numerical schemes which can be used for the PDEs, attempts to approximate the RPIEs are generally not very successful, and such schemes are often found to be low order accurate and exponentially unstable at high frequencies.

We describe how 'stability coefficients' can be computed for RPIE approximation schemes and how they are used to determine a scheme's stability. We also discuss ways of designing more accurate schemes and illustrate both points with numerical test results.

STABILITY OF FULLY DISCRETE SPECTRAL-COLLOCATION METHODS IN THE NUMERICAL SOLUTION OF CONVECTION-DIFFUSION PROBLEMS

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

In this talk we investigate the stability of fully discrete spectral-collocation methods for solving convection-diffusion equations of the form

$$u_t(x, t) = au_{xx}(x, t) - u_x(x, t), \quad -1 < x < 1, \quad t > 0$$

with appropriate initial- and boundary conditions (a is a positive constant). After discretization of this initial-boundary value problem with respect to the space variable x , one obtains a system of ordinary differential equations which will be solved by a one-step method in time (e.g. the classical Runge-Kutta method). Stability of the fully discrete process is investigated by studying the eigenvalues and the resolvent of a matrix related to the system of ordinary differential equations. Investigating stability of fully discrete processes by using resolvents has recently been done by Lenferink & Spijker, Reddy & Trefethen and others.

APPROXIMATION OF LATTICE EQUATIONS

D. B. Duncan (Heriot-Watt University)

We describe how numerical approximation techniques can shed some light on the properties of Toda lattice type systems of Hamiltonian ODEs. Amongst other things, these equations are used to model chains of atoms, where each atom interacts only with its nearest neighbours. These lattice equations look very much like time dependent PDEs discretised in space only, and, in a reversal of the standard practice, information can be obtained by approximating the ODE system by a PDE. This is done in the equivalent of the fine mesh limit using Taylor expansions. There are also travelling solitary wave

solutions which are not described well by the fine mesh asymptotics, but qualitative and quantitative information about them can be obtained by variational methods akin to Galerkin methods. Finally, the interaction and stability of the travelling waves can be studied using a symplectic ODE solver.

INEXACT AND PRECONDITIONED UZAWA ALGORITHMS FOR SADDLE POINT PROBLEMS Howard C. Elman (University of Maryland, USA)

We develop and analyze variants of the Uzawa algorithm for solving symmetric indefinite linear systems of the type arising from discretization of the Stokes equations. Each step of this algorithm requires the solution of a symmetric positive-definite system of linear equations. We prove that if this computation is replaced by an approximate solution produced by an arbitrary iterative method, then with relatively modest requirements on the accuracy of the approximate solution, the resulting inexact Uzawa algorithm is convergent with convergence rate close to that of the exact algorithm. In addition, for mixed finite element discretizations of the Stokes equations, we show how to precondition the system using a submatrix of the pressure mass matrix so that convergence of both the exact and inexact Uzawa algorithms is improved. The analysis is supplemented by numerical results demonstrating the effectiveness of the inexact and preconditioned algorithms.

This work is in collaboration with Gene Golub of Stanford University.

FAST NUMERICAL SOLUTION OF THE EXTERIOR HELMHOLTZ PROBLEM BY IMBEDDING Oliver Ernst (Stanford University, U.S.A.)

The *Helmholtz* or *reduced wave* equation describes the spatial part of time-harmonic wave fields at constant propagation speed. In acoustic or electromagnetic scattering problems, the wave field resulting from the interaction of a physical obstacle, the scatterer, with some given incident wave is sought. This requires solving the Helmholtz equation

$$-\Delta u - k^2 u = f$$

on the (unbounded) domain D exterior to the scatterer. Here, $k \in \mathbb{R}$ is the wave number and f is a source term. A unique solution to this equation is specified by imposing the asymptotic condition

$$\lim_{r \rightarrow \infty} r^{\frac{d-1}{2}} (u_r - iku) = 0$$

known as the Sommerfeld radiation condition, r denoting the radial coordinate and d the dimension of the underlying space.

When the infinite domain is truncated for numerical computation, this introduces a new, artificial boundary B on the computational domain. It then becomes crucial to accurately incorporate the radiation condition into the finite-domain problem. This has recently been solved by Keller and Givoli, using an explicit representation of the *Dirichlet-to-Neumann* (DtN) mapping, which applies to circular or spherical artificial boundaries in two or three dimensions, respectively. The DtN boundary condition is exact, i.e. the solution of the problem formulated with the DtN boundary condition is the restriction of the solution of the unbounded-domain problem to the computational domain, which is as good as one can do.

This talk describes an algorithm that applies the classical fast-Poisson solver type approach to the exterior Helmholtz problem. We will describe the linear system of equations that arises when the Helmholtz equation is discretized on a truncated domain using finite

differences as well as how the DtN formulation can be combined with fast solvers based on the fast Fourier transform and cyclic reduction techniques.

DECUHR: AN ALGORITHM FOR AUTOMATIC INTEGRATION OF SINGULAR FUNCTIONS OVER A HYPERRECTANGULAR REGION

Terje O. Espelid (University of Bergen) & *Alan Genz* (Washington State University, USA).

We describe an automatic cubature algorithm for functions that have a singularity on the surface of the integration region. The algorithm combines an adaptive subdivision strategy with extrapolation. The extrapolation uses a non-uniform subdivision that can be directly incorporated into the subdivision strategy used for the adaptive algorithm. The algorithm is designed to integrate a vector function over an n -dimensional rectangular region and a FORTRAN implementation is included. We will illustrate the use of the code on a several examples.

PARALLEL GLOBALLY ADAPTIVE QUADRATURE ON THE KSR-1

T. L. Freeman (University of Manchester)

We consider the problem of approximating, on a parallel computer, the one-dimensional definite integral

$$I = \int_a^b f(x)dx,$$

to some given absolute accuracy ϵ .

We have implemented five algorithms that exploit parallelism at different granularities on the KSR-1 parallel computer. The most successful algorithm is one that is dynamically adaptive and exploits parallelism by concurrent applications of the underlying quadrature rule.

CONVERGENCE RATES FOR POLYNOMIAL INTERPOLATION OF ANALYTIC FUNCTIONS

B. Fornberg (Exxon Research Corp, USA)

Problems with polynomial interpolation of high orders are well known. The convergence/divergence rates depend on the functions that are interpolated and on how the interpolation nodes are distributed. A both complete and very simple theory for this has existed for decades - unfortunately in places and forms quite inaccessible to most numerical analysts. In this presentation, this theory will be explained through a series of illustrations.

SOME PRACTICAL EXPERIENCE WITH THE TIME INTEGRATION OF THE NONLINEAR GALERKIN METHOD

B. García-Archilla (Universidad de Valladolid, Spain)

A number of promising ideas have recently been suggested for the numerical integration of dissipative partial differential equations. Part of the recent literature on the subject has aimed at obtaining theoretically sound, time-saving adaptive procedures to discretise the spatial derivatives. The nonlinear Galerkin method is a prominent instance of this. However, little attention has been paid to efficient integration in time. In most cases, time-stepping methods of low accuracy are coupled with sophisticated discretizations in space. We present some numerical experiments comparing the performance of proposed implementations of the new techniques for spatial discretization with that of standard

methods coupled with efficient (but already available) time integrators for ordinary differential equations. It turns out that these time integrators can improve efficiency by several orders of magnitude with respect to methods currently used.

NUMERICAL SOLUTION OF NON-CONVEX GINZBURG-LANDAU VARIATIONAL PROBLEMS

A R Gardiner (University of Sussex)

Non-convex Ginzburg-Landau energy functionals arise in the modelling of Phase transformations and superconductivity. These give rise to semi-linear elliptic equations, possibly after a time discretisation of semi-linear parabolic equations. In this talk the numerical solution of these elliptic equations is discussed. In particular we look at the computational issues arising in the study of Phase field equations and minimisation vector Ginzburg-Landau energy functionals.

A NON-LINEAR SECOND-ORDER METHOD FOR SOLVING ODES

R Garrapa (University of Bari, Italy)

We consider the IVP

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0.$$

In order to find an approximation of the solution $y(t)$, we consider an arbitrary value of $\beta \in \mathbb{R}$ and divide the equation by $y(t) + \beta$ so that it becomes

$$\frac{y'(t)}{y(t) + \beta} = \frac{f(t, y(t))}{y(t) + \beta}$$

which is equivalent to

$$\frac{\partial}{\partial t} \ln(y(t) + \beta) = \frac{f(t, y(t))}{y(t) + \beta}.$$

Integrating this relation over the interval (t_n, t_{n+1}) and approximating the right hand side by a convex combination of its values at the ends of the interval, we obtain

$$(y_{n+1} + \beta) \exp\left\{-\theta h \frac{f(t_{n+1}, y_{n+1})}{y_{n+1} + \beta}\right\} = (y_n + \beta) \exp\left\{(1 - \theta)h \frac{f(t_n, y_n)}{y_n + \beta}\right\},$$

where $h = t_{n+1} - t_n$ and $0 \leq \theta \leq 1$. It may be shown that the method is consistent of order two if $\theta = 1/2$ or if β is chosen in an appropriate manner to depend on y_n . In the latter case it is possible to have either an explicit or an implicit method of order two.

ITERATIVE METHODS FOR THE DETECTION OF HOPF BIFURCATIONS IN FINITE ELEMENT DISCRETISATIONS OF INCOMPRESSIBLE FLOW PROBLEMS

T. J. Garratt (AspenTech UK) *K. A. Cliffe* (AEA Technology) & *A. Spence* (University of Bath).

This talk is concerned with the problem of computing a small number of eigenvalues of large sparse generalised eigenvalue problems arising from mixed finite element discretisations of time dependent equations modelling viscous incompressible flow. The eigenvalues of importance are those with smallest real part and can be used in a scheme to determine the stability of steady state solutions and to detect Hopf bifurcations. We introduce a modified Cayley transform of the generalised eigenvalue problem which overcomes a drawback of the usual Cayley transform applied to such problems. The subspace iteration method is then applied to the transformed eigenvalue problem to compute approximations to the eigenvalue of smallest real part. Numerical experiments are performed

using the models of double diffusive convection, flow over a backward facing step, and flow past a cylinder.

OPTIMIZATION OF AN INVERSE SIESMIC PROBLEM

Susana Gomez (INRIA Rocquencourt, France & University of Mexico)

For oil prospection purposes, acoustic parameters have to be estimated to fit (in the least squares sense), the solution of a wave equation 2-D model to data. This data measures the acoustic response of the earth to one or several explosive sources.

We will show why the least squares structure can not be used, and how the problem can be reformulated to avoid the use of global optimization methods, an unthinkable possibility due to the cost of the objective function (more than 100 Cray2-seconds).

A limited memory Quasi-Newton method is used in a Cray2 to optimize the bounded velocities in a multiscale basis (information is not needed in all points of the grid, so the dimension of the problem goes from 12 to 2000 optimization parameters) and the impedances in the full grid (up to 70000 variables). Numerical results will be given.

IS SOR BEING REVIVED?

P.R. Graves-Morris (University of Bradford)

Recent work by Dancis [1991] has shown that the performance of SOR acceleration using so-called optimal polynomial acceleration can be substantially improved. Eiermann and Varga [1993] re-examined the theoretical basis of the derivation of ω_{opt} , and showed how the discrete character of the spectrum of the iterated operator must be incorporated as an essential ingredient of the new and evolving theory.

The selection of ω is more natural in the framework of non-linear methods, such as the vector epsilon algorithm, in which the eigenvalues of the iterated operator appear as poles of the generating (or transfer) function, and ω turns out to be the same as that recommended by Dancis.

By using the vector epsilon algorithm (or related methods), the effect of the leading eigenvalues of the iterated operator is automatically taken into account [Graves-Morris, 1992], and this feature necessarily follows from the theorems of Graves-Morris and Saff [1988] or more directly from that of Matos [1992]. Recent numerical work by da Cunha and Hopkins [1991/3] confirms the theoretical predictions, addresses the problem of how ω should be chosen in practice and of how the computations can be parallelised for greater efficiency.

After reviewing the status of the recent theoretical developments mentioned above, the talk will focus on current progress with the theoretical basis of acceleration of convergence of vector sequences of SOR type.

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J. Dancis, 1991, Diagonalising the SOR iteration method, SIAM J Matrix Anal. Appl. 12, 661-678.

J. Dancis, 1991, The optimal ω is not best for the SOR iteration, Lin. Alg. Appl. 154-156, 819-845.

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P.R. Graves-Morris and E.B. Saff, 1988, Row convergence theorems for generalised inverse vector-valued Padé approximants, J. Comp. App. Math. 23, 63–85.

A.C. Matos, 1992, Convergence and acceleration properties of the vector ϵ -algorithm, Num. Algs 3, 313–320.

KRYLOV SUBSPACE METHODS FOR THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

Richard Hanby (UMIST)

Schemes such as the SIMPLE algorithm are often used to solve the discrete Navier-Stokes equations. However, the decoupling of momentum and continuity equations involved means that convergence of rotationally dominated problems is often slow and can lack robustness.

Modern computer architectures mean that it is feasible to attempt to solve coupled Navier-Stokes systems (which are sparse, unsymmetric, indefinite and singular) using conjugate gradient type methods such as the quasi-minimal residual (QMR) method.

In this talk I compare the effectiveness of some Krylov subspace methods for this class of problem and present some numerical results.

THE EVALUATION OF WAVELET INTEGRALS

David Handscomb (Oxford University)

Multiresolution wavelets of compact support offer a powerful tool for solving differential equations by Galerkin-type methods, particularly when shock or boundary-layer phenomena call for high resolution in a small region. The implementation of this technique calls for the evaluation of integrals of products of such wavelets, their derivatives, and other functions (such as polynomials). When the problem is posed on a finite region, it may call also for the values of the same integrals when the range of integration is truncated at one or both ends. We show that a great many of such integrals may be evaluated exactly by linear algebra.

THE MATRIX SIGN DECOMPOSITION AND ITS RELATION TO THE POLAR DECOMPOSITION

Nicholas J. Higham (University of Manchester)

The sign function of a square matrix was introduced by Roberts in 1971. We show that it is useful to regard $S = \text{sign}(A)$ as being part of a matrix sign decomposition $A = SN$, where $N = (A^2)^{1/2}$. This decomposition leads to the new representation $\text{sign}(A) = A(A^2)^{-1/2}$. Most results for the matrix sign decomposition have a counterpart for the polar decomposition $A = UH$, and vice versa. To illustrate this, we derive best approximation properties of the factors U , H and S , determine bounds for $\|A - S\|$ and $\|A - U\|$, and describe integral formulas for S and U . We also derive explicit expressions for the condition numbers of the factors S and N . An important equation expresses the sign of a block 2×2 matrix involving A in terms of the polar factor U of A . We apply this equation to a family of iterations for computing S by Pandey, Kenney and Laub, to obtain a new family of iterations for computing U . The iterations have some attractive properties, including suitability for parallel computation.

NONLINEAR STABILITY THEORY FOR ODES: T-STABILITY, AN ASYMPTOTIC APPROACH

A.R. Humphries (University of Bristol)

A new nonlinear stability concept, T-stability, is introduced. The classical nonlinear stability theories, G-stability for one-leg methods and B-stability for Runge-Kutta methods, are both defined in terms of the step by step behaviour of the numerical solution. However, when approximating the long time behaviour of a dynamical system it is the *asymptotic behaviour* of the numerical solution that is of importance, not its step by step behaviour. Continuous systems possessing a unique fixed point and a strictly negative one-sided Lipschitz constant are considered; this implies that all trajectories converge to the fixed point and a method is said to be T-stable if for any such problem and any fixed step-size the numerical solution (if it exists) converges to the fixed point. Since the linear test problem also has this form it follows that every T-stable method is A-stable. Dahlquist's G-stability theory is used to show that for both one-leg *and* linear multistep methods, an irreducible method is T-stable if and only if it is A-stable. It is shown that every algebraically stable Runge-Kutta method is T-stable. A complete characterization of the T-stable Runge-Kutta methods has not been found, but it is shown that the trapezoidal rule which is not algebraically stable (unless viewed as a general linear method) is T-stable, so that T-stability encompasses a wider class of Runge-Kutta methods than algebraic stability. More surprisingly the three stage Lobatto IIIA method (which is not algebraically stable even when viewed as a general linear method) is also shown to be T-stable. We ask (rhetorically) whether T-stability might also be equivalent to A-stability for Runge-Kutta methods.

THE NUMERICAL SPLITTING ERROR IN ADVECTION-REACTION EQUATIONS

Willem Hundsdorfer (CWI, Amsterdam)

One of the main problems in the numerical simulation of air pollution problems is the correct treatment of advection and chemical reactions. These two aspects are modeled by equations of the type

$$c_t + u \cdot \nabla c = f(c)$$

where c is a vector of chemical concentrations, u is a given wind field and $f(c)$ is a stiff, nonlinear term describing the reaction.

Assuming that we start with a suitable space discretization for $u \cdot \nabla c$, there are two well-known classes of time integration methods for the convection part of the above equation, namely multistep Adams methods and one-step explicit Runge-Kutta methods.

On the other hand, due to stiffness, the chemical reaction part should be integrated with some implicit scheme. Full use of an implicit integrator on the complete equation would give rise to huge systems of algebraic equations with coupling between all grid points and all chemical components. In order to avoid this, one usually employs *splitting* of the equation, where first the convection part is solved on a small time interval with an explicit method, followed by solution of the chemical reactions on the same interval with an implicit scheme.

In this talk we shall consider the error introduced by such splitting procedures, in combination with Adams and Runge-Kutta methods for the convection part of the equation.

THREE-DIMENSIONAL FLUID FLOW IN A TUBE USING FINITE AND PSEUDOSPECTRAL DISCRETISATIONS

R. Hunt (Strathclyde University)

A numerical solution of the flow of a steady incompressible fluid in a generalised tube with arbitrary cross-section and centre-line is presented for Reynolds up to 1000. The physical domain is transformed onto either a rectangular parallelepiped or a circular cylinder. The Navier-Stokes equations are differenced using standard second order differences along the tube but with pseudospectral/spectral differences in the two transverse directions. The use of such differences in the transverse plane greatly reduces the number of nodes required for given accuracy. The resulting algebraic system is solved using Newton iteration and can be performed on Sun Sparc workstation. Comparing results on different sized grids indicates a relative accuracy of 0.001. Cases considered include variable rectangular and elliptical cross-section tubes. Specifically these are a non-symmetric tube, a tube with small outlet area, smooth step-down and step-up wedges, a variable elliptical cross-section tube and a circular tube in the shape of an hyperbola. The resulting flows display novel three-dimensional features not present in two-dimensional flows.

THE NUMERICAL COMPUTATION OF ZEROS OF BESSEL FUNCTION $J_\nu(z)$ REGARDED AS A FUNCTION OF ν FOR ANY GIVEN REAL OR COMPLEX z

Yasuhiko Ikebe (University of Tsukuba) Nobuyoshi Asai (University of Tsukuba) Yoshinori Miyazaki (University of Tsukuba) DongSheng Cai (University of Tsukuba) & Issei Fujishiro (Ochanomizu University).

John Dougall [Proc. Edin. Math. Soc. 18 (1900), 33-83] appears to be the first one to encounter the need of studying the zeros of $J_\nu(z)$ as a function of ν for a given z (in fact, his case was such that z is positive pure imaginary). In 1936, Jean Coulomb [Bull. Sci. Math 60(1936), 297-302] studied the same problem much more extensively but apparently unaware of Dougall's work.

More recently, P. Flajolet and R. Schott [Europ. J. Combinatorics 11 (1990), 421-432] obtain in their study of a certain combinatorial problem the Mittag-Leffler expansion

$$J_{\nu-1}(2)/\{\nu J_\nu(2)\} = 1 + \sum_{r \geq 0} c_r/(\nu - \zeta_r),$$

where the ζ_r are the zeros of $J_\nu(2)$ as a function of ν and the c_r are constants. P. Feinsilver and R. Schott [Math. Comp. 59 (1992), 153-156] compute approximate values of the first several zeros of $J_\nu(2)$ by computing the corresponding zeros of Lommel polynomials of various order m (in fact, $m = 4, 5, \dots, 15$) and give an asymptotic error estimate which involves the derivative of the form $dJ_{\nu-1}(2)/d\nu$; but no indications are given of their actual numerical procedure.

In this work, we will present a straightforward matrix algorithm for solving $J_\nu(z) = 0$ for any given $z \neq 0$, real or complex, as described in the following theorem:

Theorem Let $z \neq 0$ be a given real or complex number and let T_n be the symmetric tridiagonal matrix of order $n = 1, 2, \dots$, defined by

$$T_n = \begin{bmatrix} -1 & z/2 & & 0 \\ z/2 & -2 & \ddots & \\ & \ddots & \ddots & z/2 \\ 0 & & z/2 & -n \end{bmatrix}.$$

Then, if $J_\nu(z) = 0$ there is a sequence of eigenvalues ν_n of T_n such that $\nu_n \rightarrow \nu$. Conversely, if a sequence of eigenvalues ν_n of T_n converges to a limit, say ν , then $J_\nu(z) = 0$. The following asymptotic error estimate is found to be valid:

$$\nu - \nu_n = (z/2)J_{\nu+n}(z)J_{\nu+n+1}(z)(1 + o(1))/\sum_{k=1}^{\infty} J_{\nu+k}^2(z).$$

The eigenvalues of T_n are precisely the zeros of the Lommel polynomial $R_{n,\nu}(z)$ regarded as a function of ν .

The theorem offers many useful applications, and a few of them will be demonstrated.

SOLUTION OF FUNCTIONAL EQUATIONS BY DIRICHLET SERIES

A. Iserles (University of Cambridge)

Dirichlet series have been known in number theory since the pioneering work of Hardy and Riesz but it seems that they have escaped the attention of numerical analysts. In this talk I commence by demonstrating how to expand the solution of delay equations of neutral type, of the form $y'(t) = Ay(t) + By(qt) + Cy'(qt)$, where A , B and C are square matrices and $q \in (0, 1)$, into Dirichlet series. This provides a means to model the solution for a very long time with assured, realistic (and small!) error bounds and is clearly superior to time-stepping algorithms.

Next, we review recent work in solving functional equations of advanced type, $y'(t) = f(y(t), y(qt))$, where f is appropriately smooth and $q > 1$. Again, Dirichlet series are at the centre of an effort to determine analytic features of such equations and to model them numerically. A recursive definition of this series requires graph theory and their analysis calls for a mixture of algebraic combinatorics and analytic function theory.

It is known that functional equations exhibit a wealth of intricate dynamical phenomena. However, the analysis of functional equations is at its infancy. Careful numerical modelling is important not just in applications but also on the pure mathematical side, to gather information on what to prove and how!

SYMPLECTIC PARTITIONED RUNGE-KUTTA METHODS FOR CONSTRAINED HAMILTONIAN SYSTEMS

Laurent Jay (Université de Genève, Switzerland)

This article deals with the numerical treatment of Hamiltonian systems with holonomic constraints. A class of partitioned Runge-Kutta (PRK) methods, consisting of the couples of Lobatto IIIA and Lobatto IIIB methods, has been discovered to solve these problems efficiently. They are the first known methods which possess the following features: Firstly, they are symplectic, a desirable property for the long-time integration of Hamiltonian systems. Secondly, when applied to semi-explicit differential-algebraic equations (DAE's) of index 3, including Hamiltonian systems with holonomic constraints, the numerical solution can be naturally defined in order to remain consistent with all underlying constraints, without destroying the symplecticity of the method. Thirdly, their order of convergence is unchanged when applied to semi-explicit index 3 DAE's. Thus these methods show clearly their superiority in terms of symplecticity and convergence compared to known numerical methods. Numerical examples have been performed which illustrate the theoretical results.

ON IOM(q): INCOMPLETE ORTHOGONALIZATION METHODS FOR LARGE UNSYMMETRIC LINEAR SYSTEMS

Zhongxiao Jia (Universität Bielefeld, Germany)

Incomplete orthogonalization methods, IOM(q), proposed by Saad have become quite popular for solving large unsymmetric linear systems, and many people have used them. As is well known, however, their convergence behaviors have not yet been understood. In fact, no theory of convergence on IOM(q) has been given. In this paper, we analyze in detail IOM(q) from theoretical point of view, and establish their theory of convergence, in which we derive some important relationships showing how the unsymmetry of the matrix A and the parameter q involved in IOM(q) impose effects on IOM(q) and clarify those prevailing realisations. The results expose why IOM(q) are usually more suitable than full orthogonalization methods (FOM) but have the risk of potential failure when A is nearly symmetric.

Meanwhile, we discuss IOM(q) for general cases and, surprisingly, show that IOM(q) usually work well though they are more possibly subject to failure. In conclusion, we disprove a conjecture of Saad: IOM(q) may converge in general, provided that q is sufficiently large. As for practical considerations, we suggest one strategy of choosing the parameter q . Preliminary experiments show that IOM(q) are quite efficient and competitive with FOM, in particular when A is nearly symmetric.

ON MESH ADAPTIVITY FOR TIME-DEPENDENT PROBLEMS

Peter K. Jimack (University of Leeds)

When numerically solving time-dependent partial differential equations whose solutions may contain regions of rapid change over small length-scales, some form of spatial adaptivity is often required. This talk will begin with a very brief outline of two adaptive methods: h -refinement and unrefinement of the spatial mesh and r -refinement or relocation of the spatial mesh. A hybrid method which considers how these approaches might be combined to best advantage for certain 2-d problems (in space) will then be discussed. The particular examples which will be considered in the talk are nonlinear convection-diffusion equations of the form

$$\frac{\partial u}{\partial t} + ku + \nabla \cdot (c(u, \underline{x})u) - \epsilon \Delta u = f$$

and certain phase-field equations which, in their simplest form, may be expressed as the coupled system

$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial \phi}{\partial t} = K \Delta u$$

and

$$\alpha \xi^2 \frac{\partial \phi}{\partial t} = \xi^2 \Delta \phi + \frac{1}{2a} (\phi - \phi^3) + 2u .$$

For certain values of the key parameters in these types of problem it is known that the solutions have steep fronts which may move through the spatial domain with time. Hence the use of adaptivity can lead to enormous savings in computational effort -- which will be demonstrated.

EXPERIMENTS WITH A HESSIAN-FREE METHOD FOR SPARSE MINIMAX PROBLEMS

Kristjan Jonasson (The Technical University of Denmark)

An algorithm for sparse nonlinear minimax problems will be presented. The algorithm is based on trust regions and sequential linear programming and it is globally convergent. On each iteration a linear programming problem is solved for a basic step. If necessary this is followed by the determination of a minimum norm corrective step, based on a first order Taylor approximation. No Hessian information needs to be stored. A sparse implementation of the method has been programmed in FORTRAN 77 and tried on several example problems, including some from the new CUTE collection of test problems. We shall show some of the results, along with comparison with some other methods.

We shall also present a modification of the method where we combine the trust region approach and conjugate gradients to speed up the convergence. The resulting method is also globally convergent and Hessian free, but somewhat more complicated than the first.

A VOLTERRA INTEGRAL TYPE METHOD FOR SOLVING INITIAL-BOUNDARY VALUE PROBLEMS WITH NONLINEAR BOUNDARY CONDITIONS

B. Jumarhon (University of Strathclyde) & S. McKee (University of Strathclyde).

In analytical investigation into initial-boundary value problems, a common strategy is to seek an integral equation reformulation which can be used to resolve questions such as existence, uniqueness and stability of solutions. However, the possibility of using the integral equation reformulation to obtain a numerical solution of the initial-boundary value problem does not appear to have been fully exploited. In this talk, two examples will be presented to illustrate the feasibility of solving some initial-boundary value problems with nonlinear boundary conditions by treating their equivalent systems of Volterra integral equations. In the first example, a coupled system of first and second kind singular Volterra integral equations will be set up for an initial-boundary value problem with nonlinear boundary conditions, and for the system of integral equations the associated product integration schemes will be given. In the second example, the equivalent system of nonlinear Abel-Volterra equations of the second kind will be derived for an initial-boundary value problem with more complicated nonlinear boundary conditions, where the nonlinearity does not satisfy a global Lipschitz condition. The method of truncating out singularities will be employed to this problem to obtain high order product integration schemes. A different approach from the standard method of proving convergence for Volterra integral equations of the second kind will be used to overcome the difficulties due to the complicated nonlinearity. Also in this example, some theoretical understanding of the solution of the initial-boundary value problem will be obtained by consideration of the system of Volterra integral equations.

NUMERICAL SOLUTION OF HAMILTONIAN NORMAL FORMS

B. Karasözen (Middle East Technical University, Turkey)

Hamiltonian equations in the normal form

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad \dot{q}_k = \frac{\partial H}{\partial p_k}, \quad k = 1, 2, \dots$$

$$H = \sum_{k=1}^n \omega_k \rho_k + \frac{1}{2} \sum_{j,k=1}^n \omega_{jk} \rho_j \rho_k \quad \text{with} \quad \rho_k = \frac{1}{2}(p_k^2 + q_k^2)$$

are considered for comparison of different symplectic integrators. Implicit mid-point rule, a symplectic DIRK method, fully implicit Runge-Kutta methods with real spectra of the coefficient matrix A and methods based on a Runge-Kutta ansatz for generating functions are investigated. The resulting nonlinear algebraic equations are solved by Newton-Raphson or fixed point iteration. It turns out that a symplectic integrator with an iterative method for the solution of implicit equations has to be considered as a new ode solver, which may or may not be symplectic, depending on the number of iterations. The effectiveness of the methods are compared with respect to order, stability and cost by presenting various numerical results.

SOLUTIONS TO LARGE SYLVESTER EQUATIONS USING THE ARNOLDI AND GMRES METHODS

Ebrahim M. Kasenally (Imperial College) & Imad M. Jaimoukha (Imperial College). This paper focuses on efficient algorithms for solving Sylvester equations of the form $AP + PB + cd' = 0$ in which c and d are vectors. We consider two Krylov subspace methods for calculating low rank approximate solutions to these equations, namely, the Arnoldi [Saad, Math. Comput., Vol 37, No 155, pp 105-126, 1981] and the Generalised Minimum Residual (GMRES) [Saad and Schultz, SIAM J. Sci. Stat. Comput., Vol 7, No 3, pp 856-869, 1986] methods. Each is exploited to yield a low rank approximate solution in terms of the solution to a low dimensional linear matrix equation, furthermore, we derive exact, low dimensional expressions for the residual errors incurred. We discuss the numerical solution of the low dimensional linear matrix equation which arises from the GMRES method and present an algorithm for its solution. All the results obtained are then extended via the block Arnoldi process to tackle the solution of $AP + PB + CD' = 0$ in which C and D have more than one column.

IMPLICIT RUNGE-KUTTA METHODS FOR SINGULARLY PERTURBED INTEGRODIFFERENTIAL EQUATIONS

Jean-Paul Kauthen (University of Fribourg, Switzerland)

Singularly perturbed Volterra integral and integrodifferential equations arise in many physical and biological problems. From the numerical point of view, such equations have received only little attention while convergence properties of numerical methods for singularly perturbed ordinary differential equations are now well understood.

We consider singularly perturbed Volterra integrodifferential equations of the following forms

$$\epsilon z'(t) = f(t, z(t)) + \int_0^t k(t-s)g(s, z(s))ds, \quad z(0) = z_0, \quad \text{and}$$

$$\epsilon z'(t) = f(t, z(t)) + \int_{-\infty}^t k(t-s)g(z(t), z(s))ds, \quad z(t) = g(t), -\infty < t \leq 0,$$

where $0 \leq \epsilon \ll 1$, $t \in [0, T]$ and f, k and g are sufficiently smooth functions.

We analyse the convergence properties of extended implicit Pouzet-Volterra-Runge-Kutta methods applied to the above equations as well as to the associated integrodifferential-algebraic systems. It will be shown that the numerical solution and the corresponding error have ϵ -expansions like the exact solution. It will turn out that the coefficients in the expansion of the error are the errors of the Runge-Kutta method applied to the integrodifferential-algebraic systems which determine the coefficients in the expansion of the exact solution.

ON CHAOTIC BEHAVIOUR OF SOME DIFFERENCE EQUATIONS

S Keras (University of Cambridge)

We investigate the following difference equation

$$y_{n+1} = 2y_n - y_{n-1} - \lambda g(y_n).$$

It is proved that when the function $g(x)$ has two simple zeroes, then for sufficiently large λ the solution of the equation has a horseshoe, hence not suitable for numerical calculations. We also prove that when the function $g(x)$ does not have two real zeroes, there is no chaotic behaviour.

MATRIX POWERS IN FINITE PRECISION ARITHMETIC

Philip A. Knight (University of Manchester)

In exact arithmetic, the k th step of stationary iteration for solving a linear system $Ax = b$ can be written in matrix form as $Mx_{k+1} = Nx_k + b$, where $A = M - N$ and $\{x_i\}$ is the set of iterates. Clearly if $e_k = x_k - x$ is the error in the k th iterate then, letting $G = M^{-1}N$, $e_k = G^k e_0$, and so the intermediate and limiting convergence behaviour of the system is governed by the growth of the powers of G .

Our aim is to understand the behaviour of matrix powers in floating point arithmetic in the hope that this will increase our understanding of the effect of rounding errors on the convergence properties of stationary iteration and other processes where matrix powers play a key role.

Initially we examine the behaviour of matrix powers in exact arithmetic. In particular, we review a number of methods of obtaining bounds on the norms of their powers. We then examine how the Jordan canonical form of a matrix can be used to model the effects of rounding error to obtain conditions that ensure that the correct asymptotic behaviour is preserved and for certain special cases we can bound the size of $fl(A^k)$ for finite values of k . We also show that for certain matrices our bounds are very tight. Finally we find a direct link between the pseudoeigenvalues of a matrix and the behaviour of $fl(A^k)$.

ANTI-GAUSSIAN QUADRATURE FORMULAS

Dirk P. Laurie (Potchefstroom University for Christian Higher Education, South Africa)

An anti-Gaussian quadrature formula H_{n+1} is an $n+1$ point formula of degree $2n-1$ which integrates polynomials of degree up to $2n+1$ with an error equal in magnitude but of opposite sign to that of the n point Gaussian formula G_n . The average $L_{2n+1} = (G_n + H_{n+1})/2$ is therefore a $2n+1$ point formula of degree at least $2n+1$ which contains the points of G_n as a subformula, and can be used as an alternative to the Kronrod extension K_{2n+1} of G_n . The anti-Gaussian formula H_{n+1} has positive weights, and its nodes are in the integration interval and are interlaced by those of the Gaussian formula G_n . Numerical evidence indicates that the power of the formula L_{2n+1} to integrate monomials is in practice as good as that of Kronrod formula K_{2n+1} .

The anti-Gauss-Christoffel formula $H_{n+1}^{(w)}$ corresponding to the Gauss-Christoffel formula $G_n^{(w)}$ for the weight function w over the interval $[a, b]$ has the same desirable properties, except that the nodes may or may not all be inside $[a, b]$ depending on w . The formula $H_{n+1}^{(w)}$ is as easy to compute as the next Gauss-Christoffel formula $G_{n+1}^{(w)}$. For the Gauss-Laguerre and Gauss-Hermite cases (where the Kronrod extension is known to be nonexistent), the anti-Gaussian formula exists and has all nodes inside the integration interval.

LOCAL STABILITY OF TRANSLATES OF POLYHARMONIC SPLINES IN EVEN SPACE DIMENSION

Jeremy Levesley (University of Leicester)

We are concerned with the local stability of functions on $\mathbf{R}^n$,

$$G(x) = \sum_{z \in \mathbf{Z}^n} d_z \phi(\|x - z\|),$$

where $\phi : \mathbf{R}^+ \rightarrow \mathbf{R}$. By this we mean that

$$|d_z| \leq C \sup_{x \in K} |G(x)|,$$

where K is a compact neighbourhood of the origin and C is a constant dependent only on K . We consider functions ϕ which are sums of polyharmonic splines in even space dimension, and also assume that n is even.

IMPROVING EIGENSTRUCTURE ASSIGNMENT BY A MINIMISATION TECHNIQUE

D M Littleboy (University of Reading)

We consider the problem: given matrices (A, B, C) , find a feedback matrix, K , such that $(A + BKC)$ has desired eigenvalues and corresponding eigenvectors. This is called output feedback by eigenstructure assignment.

Methods for eigenstructure assignment are applied in the aircraft industry where it is desired to assign eigenvalues and their mode output and input coupling vectors by

$$G_O = CV, \quad G_I = W^T B.$$

Here V, W^T are the modal right and left eigenvector matrices respectively.

Techniques are described for assigning exactly $p \equiv \text{rank } C$ eigenvalues and eigenvectors to achieve the desired output coupling. The input coupling vectors obtained by this process are generally not satisfactory. A novel minimisation algorithm is derived to improve the feedback design based on the structure of the aircraft problem.

STABILITY ANALYSIS OF THE θ -METHODS FOR NEUTRAL DIFFERENTIAL EQUATIONS

Yunkang Liu (University of Cambridge)

The θ -methods for the numerical solution of the neutral differential equations are formulated in this paper. Two typical equations, one with constant time lag, the other with proportional time lag, are used as test equations to assess the (asymptotic) stability of the θ -methods. Global discretization errors are investigated and numerical examples are presented.

A UNITARY INTEGRATOR FOR THE MATRIX DIFFERENTIAL EQUATION $\Theta' = i\Theta\Omega(x, \Theta)$

M Marletta (University of Leicester)

The nonlinear matrix differential equation $\Theta' = i\Theta\Omega$, where Ω is a Hermitian matrix function of x and Θ , has the property that a solution matrix Θ is unitary at a point if and only if it is unitary wherever it is defined. For the solution of this equation, which arises in numerical solution of ODE eigenvalue problems, in continuous orthonormalisation for boundary value problems and in the computation of continuous SVD decompositions, it is important to use a method which preserves unitary matrices. We present one such method based on matrix exponentials and Lie products, which has performed well in applications.

POLYNOMIAL SPLINES OF EVEN DEGREE: BEST APPROXIMATION BY γ -SPLINES

M.F.G. Martins (Universidade Nova de Lisboa, Portugal)

In $K^r[a, b]$ (linear space of the real valued functions, f , defined on $[a, b]$ such that $f^{(r-1)}$ is absolutely continuous on $[a, b]$ and $f^{(r)} \in L_2[a, b]$) we define a seminorm and we consider a class of γ -splines of even degree.

We establish the conditions to be satisfied in order to obtain a b.a. of $f \in K^r[a, b]$ in that class of γ -splines (in the sense of the above seminorm).

As a particular case we obtain the best approximation by monosplines.

We also analyse the existence and uniqueness of a best approximation interpolating f on a mesh of points in $[a, b]$.

ON APPLICATIONS OF GENSMAC: A MULTIPLE FREE SURFACE CODE FOR NEWTONIAN AND NON-NEWTONIAN FLOW

S. McKee (University of Strathclyde) & M. Tomé (University of Strathclyde).

GENSMAC is based on the ideas of the marker and cell method that arose from Los Alamos in the 1960s. It, however, has an adaptive time stepping mechanism and can solve multiple free surface problems in arbitrary shaped regions. Applications to be discussed include (a) manufacture of confectionery products by cavity filling (b) jet buckling and (c) non-Newtonian dye swell.

EXPERT SYSTEMS TO SELECT NUMERICAL SOLVERS FOR SECOND ORDER INITIAL VALUE PROBLEMS

G.V. Mitsou (University of Athens, Greece) & T.E. Simos (University of Athens, Greece).

The need to develop knowledge-based systems for scientific computing (and especially for numerical computing) has been extensively discussed in several workshops and conferences.

The numerical solution of the special second order initial value problems (SSOIVPs) has been the subject of great activity, the aim being to achieve a fast and reliable algorithm that generates a numerical solution. A result of this activity is the wide range of numerical software for solving SSOIVPs. So, it has become increasingly difficult for users to select the most appropriate package to solve their problem. Application of an inappropriate method produces incorrect results or large errors, often at the cost of highly inefficient computations.

In this paper we describe the necessary parts of an expert system for the numerical solution of the initial value problem

$$y''(x) = f(x, y), \quad y(x_0) = y_0, \quad y'(x_0) = y'_0, \quad x \geq x_0.$$

We discuss (i) the expertise to select the appropriate solver, (ii) the capability to investigate certain critical properties such as linearity, stiffness, the behaviour of the solution (oscillatory or non-oscillatory) of a given problem with minimal help from the user. Also, we will describe the basic components of an intelligent solver selector which are (1) the user interface, (2) the investigator of numerical properties (3) the knowledge base in which the numerical properties and the data base of the numerical methods have been correlated and make some recommendations of the appropriate method.

AN EXPERT SYSTEM FOR THE NUMERICAL SOLUTION OF THE RADIAL SCHRÖDINGER EQUATION

G.V. Mitsou (University of Athens, Greece) & T.E. Simos (University of Athens, Greece).

We describe the necessary parts of an expert system for the numerical solution of the radial Schrödinger equation $y'' + f(r)y(r) = 0$, where $0 \leq r < \infty$ and $f(r) = E - l(l+1)/r^2 - V(r)$. We call the term $l(l+1)/r^2$ the *centrifugal potential* and the function $V(r)$ the *potential*. If $E > 0$ we have the so-called *open-channel* problem. The problem is either to determine the phase shifts $\delta(E)$ or find those eigenvalues (resonances) E_i for which $\delta(E_i) = \pi/2$. If $E < 0$ we have the so-called *bound state problem* which is an eigenvalue problem.

We will discuss (1) the ability to solve the eigenvalue, the resonance and the phase shift problem of the radial equation and to select the appropriate family of methods and the appropriate method from the family, (2) the capability to investigate certain critical properties of the method such as how much exponential or trigonometric (i.e. which defines the trigonometric order) or Bessel and Neumann functions integrates a solver, the algebraic order, the phase-lag and the interval of periodicity of the method with minimal help from the user. We then describe the basic components of an intelligent solver selector.

COMPUTING THE GLOBAL STRUCTURES IN DYNAMICAL SYSTEMS

G. Moore (Imperial College, London)

We present a geometric approach to the computation of periodic solutions, homo/heteroclinic orbits, invariant tori and (un)stable manifolds of fixed points for autonomous systems and of invariant curves for periodically forced problems.

NON-SYMMETRY IN THE MODELLING OF CONTAMINANT TRANSPORT IN POROUS MEDIA

K.J.Neylon (University of Reading)

A model for variable-density contaminant transport in porous media is presented, together with a computational algorithm for approximating the solution. Causes of non-symmetry in the resulting linear systems are highlighted.

An example of a non-symmetric system is generated by using an implicit Taylor-Galerkin method to discretise the contaminant continuity equation in the model; this system is solved using the Bi-CGSTAB iterative method.

The performance of the algorithm is examined on two test cases from the literature.

PSEUDOSPECTRAL CHEBYSHEV METHODS FOR THE SOLUTION OF THE KDV EQUATION DOMAIN-DECOMPOSITION TECHNIQUES

F.Z. Nouri (University of Annaba, Algeria)

A study of domain-decomposition techniques for pseudospectral Chebyshev methods for the solution of the KDV equation.

A GENERALIZED ORTHOGONALITY RELATION FOR MULTIDIMENSIONAL WAVELETS

Gerhard Opfer (University of Hamburg, Germany)

The so-called multi-resolution analysis gives rise to the following set of equations in $L^2(\mathbf{R})$:

$$\psi^{(j)}(x) = \sum_{k \in \mathbb{Z}^n} h_k^{(j)} \psi^{(1)}(Ax - k), \quad j = 1, 2, \dots, \ell, \quad x \in \mathbf{R}^n, \quad (1)$$

where A is in particular a nonsingular matrix with integer entries and $\ell = |\det(A)| \geq 2$. Usually, $\psi^{(1)}$ is denoted by φ and called *scaling function* whereas the $\psi^{(j)}$, $j \geq 2$ are called *wavelets*. If (1) is Fourier transformed, where the Fourier transform is indicated by $\widehat{}$ we obtain

$$\widehat{\psi^{(j)}}(A^T z) = H^{(j)}(z) \widehat{\psi^{(1)}}(z), \text{ where } H^{(j)}(z) = (1/\ell) \sum_{k \in \mathbb{Z}^n} h_k^{(j)} e^{-i \langle k, z \rangle}, j = 1, 2, \dots, \ell, z \in \mathbb{R}^n. \quad (2)$$

Any non-singular integer matrix A partitions $\mathbb{Z}^n$ into $\ell = |\det(A)|$ equivalence classes modulo the grid $\Gamma = A\mathbb{Z}^n$. If the translates of the scaling function $\varphi = \psi^{(1)}$ are orthogonal, then it is known (e. g. MADYCH [1992, formula (5)]) that

$$\sum_{j=1}^{\ell} |H^{(1)}(z + 2\pi \tilde{z}_j)|^2 = 1, \quad H^{(1)}(0) = 1, \quad (3)$$

where the $\tilde{z}_j$ form a complete set of representatives of the equivalence classes modulo the *transposed* grid $\tilde{\Gamma} = A^T \mathbb{Z}^n$. Equation (3) together with a simplification already mentioned by PÓLYA & SZEGÖ (1971, p. 82, 275) is usually the key for constructing the scaling function and the wavelets. Our generalization concerns the choice of the representatives $\tilde{z}_j$ which in general can be selected from the equivalence classes modulo any grid of the form $G = B\mathbb{Z}^n$ where B must have certain properties. In many cases even the matrix A itself has these properties with the implication that the original grid Γ (rather than the transposed grid) can be used. As a consequence, the variety of solutions to the wavelet equations (1) is enlarged. These considerations apply, *cum grano salis*, to all of the $H^{(j)}$.

W. R. MADYCH: Some Elementary Properties of Multiresolution Analyses of $L^2(\mathbb{R}^n)$, in: C. K. CHUI (ed.) *Wavelets: A Tutorial in Theory and Applications*, 259–294, Academic Press, Boston, 1992.

G. PÓLYA & G. SZEGÖ: *Aufgaben und Lehrsätze aus der Analysis II*, 4th ed., Springer, New York, 1971, 407 p. (First edition 1925)

ON RUNGE-KUTTA DISCRETIZATIONS FOR TIME-DEPENDENT PARABOLIC PROBLEMS

Alexander Ostermann (University of Innsbruck, Austria)

We study implicit Runge-Kutta methods for the time discretization of parabolic problems of the form

$$u' + A(t)u = g(t),$$

given as initial value problems in an appropriate Hilbert space. We suppose that the linear operators $A(t)$ generate analytic semigroups. Under weak additional assumptions on $A(t)$, stability and convergence of strongly $A(\alpha)$ -stable Runge-Kutta methods will be shown.

FULL DISCRETIZATIONS OF PARABOLIC INITIAL VALUE PROBLEMS

C. Palencia (Universidad de Valladolid, Spain)

In this communication full discretizations of linear parabolic initial value problems are considered. Finite elements are used for the semidiscretization in space and a rational method is used for the semidiscretization in time. We prove the unrestricted stability of the resulting procedure in the maximum norm under very general conditions, provided that the dimension of the Euclidean space is less or equal to three.

BOUNDED HOMOTOPIES TO SOLVE SYSTEMS OF ALGEBRAIC NONLINEAR EQUATIONS

Jorge R. Paloschi (Imperial College, London)

One of the difficulties in using continuation methods to solve systems of algebraic nonlinear equations arising from chemical engineering simulation problems is the unboundness of the continuation path. When physical properties are evaluated, it is desirable that the homotopy path remains within a prescribed domain where the properties are well defined. The traditional homotopies do not guarantee a bounded path. A new family of homotopies will be proposed which have the property of bounded path within a prescribed domain. Some mathematical examples will be presented showing how the new homotopies can solve problems where the traditional ones have a path leaving a desired domain.

PARALLEL MULTIPLE SHOOTING BY PARTIAL UPDATING

A. Papini (Università di Firenze) S. Bellavia, M.G. Gasparo, M. Macconi (Università di Firenze)

We are interested in numerical solution of nonlinear TPBVP's with separated boundary conditions by multiple shooting. It is known that finite difference Newton method is generally used to solve the resulting nonlinear system $F(s) = 0$. The evaluation of the whole approximated jacobian matrix at each iteration can be extremely time-consuming, because of the involved IVP integrations.

We propose the use of iterative methods based on a partial updating strategy where only k columns of the matrix are updated and the other columns are retained from the previous iteration. In general this method requires more iterations than Newton's method. Nevertheless, it can be advantageous when integrations are the dominant cost. The given parallel scheme is designed for distributed memory architectures and can be naturally implemented on a ring topology. Numerical results obtained on a network of transputers T805-20 show the reliability and the efficiency of the proposed algorithm.

HIGH ORDER APPROXIMATIONS TO THE MATRIX EXPONENTIAL VIA OPERATOR SPLITTING

Dimpy Pathria (Princeton University, USA) & J. Bronski (Princeton University, USA). Solving the initial value problem $\dot{u} = \mathbf{H}u$ with $u(0) = u_0$, generally requires numerically exponentiating the operator $\mathbf{H}$. It is often computationally simpler however, to write $\mathbf{H} = \mathbf{A} + \mathbf{B}$ and to form the exponentials of $\mathbf{A}$ and $\mathbf{B}$. This strategy is the basis of the splitting methods, which seek to compose the exponentials of the suboperators to obtain accurate approximations to the full one. First and second order schemes have been successfully used for many years; higher order ones less so, since no such general splitting can be constructed with all positive powers of $\mathbf{A}$ and $\mathbf{B}$. By relaxing this positivity requirement, we construct here a family of splitting methods which are appropriate for solving hyperbolic problems. The k th member of the family has order $2k$ when $\mathbf{H}$ is independent of time. When $\mathbf{H}$ has a time dependence, the construction applied to a method of order $2m$ returns a method of order $2m + 1$. These convergence rates are verified through a number of numerical experiments.

NUMERICAL SOLUTION OF SECOND KIND INTEGRAL EQUATIONS ON INFINITE CYLINDRICAL SURFACES

Andrew Peplow (I.S.V.R, University of Southampton) & *Simon Chandler-Wilde* (University of Bradford).

We consider second kind integral equations, in which integration is taken over an infinite cylindrical surface of arbitrary smooth cross-section. For the purposes of implementing a numerical method a truncated version of the original integral equation is discussed. Conditions on the kernel are given which ensure invertibility and uniform boundedness of the appropriate operators. Uniform stability and convergence results for a boundary element method are obtained for an application in outdoor sound propagation over obstacles in three-dimensions. Some numerical results are presented.

ITERATIVE APPLICATION OF FFT METHODS FOR THE NUMERICAL SOLUTION OF PARTIAL DIFFERENTIAL EQUATIONS

W.M. Pickering (University of Sheffield) & *P.J. Harley* (University of Sheffield).

A method for the numerical solution of linear partial differential equations is described which involves the iterative application of FFT techniques. The general approach is to choose an equation 'near' (in some sense) to the equation to be solved and perform an iterative refinement on the solution of this 'nearby' equation. This equation is appropriately chosen from the general class of equations soluble directly by FFT methods (Le Bail, 1972) and the iteration consists of corrections to the relevant Fourier harmonic amplitudes of the solution of this 'nearby' equation.

The method is applicable to a large class of linear partial differential equations and numerical results are presented for illustrative examples of elliptic equations in the unit square with Dirichlet boundary conditions. For these problems, using a block-Jacobi iteration, it is shown that the overall operations count is $O(n^2 \log_2 n)$ for an $n \times n$ grid. Convergence rates are shown to be essentially independent of grid size and shifted iterations are employed to improve convergence rates, as in the Concus and Golub (1973) iteration. It is also shown that the new approach allows the use of a 'variable' shift which can further improve rates of convergence. The general computational behaviour of the method was found to be in good agreement with that predicted by the theoretical analysis.

ITERATIVE SOLUTION TECHNIQUES FOR THE NAVIER-STOKES EQUATIONS

Alison Ramage (University of Strathclyde) & *Andy Wathen* (University of Bristol).

The efficient solution of large systems of linear equations is of great practical importance in computational fluid dynamics. A particular example frequently encountered in industrial applications is the case of the Navier-Stokes and continuity equations for incompressible viscous fluid flow. Applying the usual mixed finite element method and a standard nonlinear solver reduces this problem to a series of nonsymmetric linear systems. These could be tackled with a nonsymmetric iteration: here, however, we adopt a different approach and take advantage of the symmetry which arises naturally in a Lagrange-Galerkin finite element discretisation.

The Lagrange-Galerkin method is a numerical technique introduced as an accurate discretisation method for advection-dominated diffusion problems. When applied directly to the time-dependent Navier-Stokes equations, it removes the nonlinearity introduced by the advection term in such a way that the resulting linear system has the character of the Stokes problem for creeping flow. Various iterative methods which have been proposed

for Stokes problems can be applied and here we compare the performance of a traditional two-level pressure correction approach with solution of the original fully-coupled indefinite problem by means of the preconditioned conjugate residual (MINRES) method. The relative performance of these algorithms will be examined both in theory and in practice. Using estimates of the eigenvalue spectrum, asymptotic estimates for the amount of work involved in implementing each method with various preconditioners can be calculated. In addition, we will present the results of practical numerical computations carried out within the framework of an industrial fluid flow simulation program (Nuclear Electric plc.'s code FEAT).

HIGH PRECISION INTEGRATION OF STIFF O.D.E'S BY MULTISTEP RADAU METHODS Stefan Schneider (Université de Genève, Switzerland)

We present an implementation of multistep collocation methods which are applicable to a large spectrum of differential problems and which are particularly useful for high precision computations. These problems include stiff differential equations, singular perturbation problems, stiff mechanical systems and D.A.E.s of index 1,2 and 3. These methods generalize one-step implicit Runge-Kutta methods as well as multistep one-stage BDF methods. We give numerical comparisons of our code with two representative codes for these methods, RADAU5 and LSODE.

INVERSE AND IMPLICIT FUNCTION THEOREMS FOR PIECEWISE DIFFERENTIABLE FUNCTIONS

Stefan Scholtes (Universität Karlsruhe, Germany)

Many numerical problems such as nonlinear complementarity problems, variational inequalities and nonlinear programming can be formulated as the problem of finding a zero of a piecewise differentiable function $f : \mathbf{R}^n \rightarrow \mathbf{R}^n$. Beside the applicability of general Newton-type algorithms, this approach provides a unified framework for sensitivity analysis and the treatment of (local or global) uniqueness questions of solutions to the above problems. The analysis of these problems makes use of inverse and implicit function theorems. We present such theorems for piecewise differentiable functions, where the emphasis lies on the following points:

- the assumptions of the theorems should impose conditions on a finite set of matrices only, thus being numerically verifiable,
- the resulting inverse or implicit function is required to be piecewise differentiable (and a fortiori locally Lipschitz continuous).

MULTIPLE SCALES ANALYSIS FOR A SPECTRAL METHOD

S.W. Schoombie (University of the O.F.S., South Africa) & E. Maré (Nedbank, South Africa).

Recently Schoombie devised a method to perform a multiple scales analysis on a finite difference scheme for the Korteweg-de Vries equation. This work is now extended to a spectral method for the Korteweg- de Vries equation, using an idea of Fornberg.

MA42 - A NEW FRONTAL CODE FOR SOLVING SPARSE UNSYMMETRIC SYSTEMS

J.A. Scott (Rutherford Appleton Laboratory) & I.S. Duff (Rutherford Appleton Laboratory).

We discuss the design and implementation of a code MA42 for solving sparse unsymmetric systems of linear equations, $Ax = b$ or $A^T x = b$, using a frontal method. A principal feature of the code is that it can solve large problems in a predetermined and relatively small amount of in-core memory since direct access data sets are optionally used for the matrix factors. The code is designed to be portable and efficient on high-performance computers. Extensive use is made of levels 2 and 3 BLAS routines. Numerical results for some practical problems are included.

CONVERGENCE RATES AND CLASSIFICATION FOR IRREGULAR FINITE ELEMENT MESHES

P.M. Selwood (University of Bristol) & A.J. Wathen (University of Bristol).

Recent advances in adaptive gridding strategies have highlighted the need to consider the Finite Element Method on irregular meshes. In this paper, we consider irregular grids in the context of refinement paths, i.e. sequences of grids such that $h \rightarrow 0$. For a two point boundary value problem with piecewise linear elements, for which $O(h^2)$ convergence is expected in the L_2 sense, we demonstrate a family of grids that give $\|u - u_h\|_{L_2} \leq Ch^p$ where p can take any value in the interval $[2, 2.5)$. Here, as usual, h is the mesh size and u and u_h are the actual and approximate solutions. Despite this apparent superconvergence, these grids actually define a sub-optimal refinement path. This is due to the high degree of irregularity of the meshes. We also propose a simple classification that discriminates when this behaviour can and cannot occur.

MULTIGRID PRECONDITIONING OF INCOMPRESSIBLE FLOW EQUATIONS

D.J. Silvester (UMIST)

Having an efficient Stokes solver is an important requisite of many Navier-Stokes solution algorithms. The Stokes operator is self-adjoint so iterative solution methods are an attractive approach for large problems. The only impediment to efficiency is the indefinite nature of the discrete system.

In this talk, some new theoretical results will be presented showing the effectiveness of V-cycle multigrid preconditioning of discrete Stokes systems. Our results apply to stable approximations of the Stokes operator, typically based on staggered grids, and also to recently developed *stabilised* approximations: equal order finite element methods or finite difference methods on unstaggered grids. We present some numerical results showing the effectiveness of our algorithm, and we compare our methodology with other multigrid preconditioners which have been proposed in the literature.

This is joint work with Andy Wathen.

THE OSCILLATORY AND PULSATILE FLOW OF A NEWTONIAN FLUID THROUGH SQUARE CORRUGATED TUBES

Z. Skalak (Institute of Hydrodynamics CAS, Czech Republic) & P. Kucera (Czech Technical University, Czech Republic).

In our contribution we describe the pulsatile and oscillatory laminar flow of a viscous Newtonian fluid through a circular infinite tube with square corrugations on its wall. At first the problem is described precisely and the existence of the solution is briefly proved for the stationary flow. Then we describe the numerical method used and discuss the results. The model studied can be applied for the blood flow through artificial vascular

grafts. In fact most of the grafts have the so called corrugations or crimps on their walls. Our long-term aim is to study the influence of the crimps of various shapes and sizes on the blood flow and suggest the geometry of the crimped wall which is the most convenient from the hydrodynamical point of view. This contribution can be understood as the first step in this direction.

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PSEUDOSPECTRAL SOLUTION OF A NONLINEAR, DISSIPATIVE SYSTEM

D. M. Sloan (University of Strathclyde) & R. Wallace (University of Strathclyde).

The aim of this work is to characterise an inertial manifold for a nonlinear, dissipative system using nodal (physical) values rather than modal (Fourier) values. The approach is illustrated using the Kuramoto-Sivashinsky (KS) equation with periodic boundary conditions in one space dimension. The KS equation is approximated using a pseudospectral discretisation in space, and the dissipativity of the resulting semi-discrete system is established. Using the concept of inertial manifolds, an algorithm is constructed which is based on the interaction between coarse grid and fine grid computations. This interaction replaces the interaction between low Fourier modes and high Fourier modes in the nonlinear Galerkin method. We shall present the results of some numerical computations on the KS equation.

ORDER CONDITIONS FOR SYMPLECTIC RUNGE-KUTTA SCHEMES

M. Sofroniou (Loughborough University) & W. Oevel (Loughborough University).

In recent years there has been much interest in the properties of Hamiltonian dynamical systems. There exists a class of methods, termed symplectic, for which the numerical integration of such systems recreates phase trajectories more faithfully than standard techniques.

It is well known that Runge-Kutta schemes are symplectic subject to the algebraic condition

$$b_i a_{ij} + b_j a_{ji} = b_i b_j, \quad 1 \leq i, j \leq s \quad (1)$$

where a_{ij} and b_j are the coefficients of the Runge-Kutta method. As a result of (1) a considerable reduction in the order conditions arises - a reduction to roughly one equation per non-rooted tree.

By parameterising (1), we will show that there exists a more natural basis for the set of necessary and sufficient order conditions; involving only $s(s+1)/2$ free parameters. Consequently, these new order conditions inherit (structurally) the properties outlined by Sanz-Serna, J. M. and Abia, L. (1991). We outline a graph theoretical process for

determining the new order conditions recursively. Furthermore we will show that *any* rooted tree arising from *same* free tree enforces the *same* algebraic constraint on the coefficients.

Finally, in the light of the above results, we re-examine the definition of the principal error function for symplectic Runge-Kutta schemes applied to Hamiltonian systems.

WAVELETS, FILTERS AND DILATION EQUATIONS

Gilbert Strang (M.I.T, U.S.A)

The search is not over! We concentrate on quadrature mirror filters, now known as wavelets. They have useful properties but substantial restrictions. The original Haar wavelet provides an example of multiresolution analysis. The Daubechies wavelets improve accuracy and smoothness but with longer support intervals (more coefficients in the dilation equation).

We will describe new "short wavelets" that come from matrix dilation equations. They are constructed from two or more scaling functions. These Geronimo-Hardin wavelets are nonzero only on two intervals. They provide self-scaling orthogonal bases for a subspace containing all piecewise linear functions and its complement. The theory involves unitary, and positive definite, matrix polynomials. Applications are predicted.

ANALYSIS OF A CELL VERTEX FINITE VOLUME METHOD FOR CONVECTION-DIFFUSION IN TWO DIMENSIONS

Martin Stynes (University of Cork, Ireland) *K.W.Morton & E.Suli* (University of Oxford)

Although the cell vertex finite volume method has been successfully applied to several challenging flow problems, the correct way of handling diffusion when the method is applied to such problems is still not universally agreed. Furthermore, the literature contains no satisfactory analysis of its behaviour in more than one dimension when diffusion is present. In this paper we address both of these issues; we design a new variant of the method for convection-diffusion problems in two dimensions and proceed to analyse this variant.

A POSTERIORI ERROR ANALYSIS FOR GALERKIN APPROXIMATIONS OF FRIEDRICHS SYSTEMS

Endre Süli (Oxford University)

The accurate and efficient resolution of localised structures, such as shocks and boundary layers, in complex multi-dimensional fluid flow problems necessitates the use of locally refined adaptive computational grids. The construction of such grids should be guided by sharp a posteriori error estimates which ensure that the adaptive algorithm is both reliable (i.e. a norm of the error is guaranteed to be below a certain tolerance) and efficient (i.e. it does not produce a grid which is overly refined).

As a first step towards developing successful adaptive algorithms for the compressible Euler and Navier-Stokes equations we derive residual-based two-sided a posteriori error bounds for Galerkin approximations of Friedrichs systems. Using a decomposition of the global error into a local part and a propagating component, we show that the graph-norm of the local component of the global error satisfies a two-sided a posteriori error bound involving the L_2 -norm of the (computable) finite element residual, and that the L_2 -norm of the error obeys an analogous two-sided bound in terms of the dual graph-norm of the residual. By concentrating on hyperbolic equations, we shall indicate the relevance

of these results in the construction of error indicators and error estimators for adaptive mesh refinement algorithms.

A BLOCK MARKOWITZ STRATEGY FOR THE SOLUTION OF SPARSE LINEAR EQUATIONS
V. Swift (University of Portsmouth, Royal Military College of Science & AEA Technology, Harwell)

Markowitz (1957) introduced a strategy for pivotal choice in the solution of sparse linear equations $Ax = b$, where A is an $n \times n$ coefficient matrix and x, b are n -vectors.

His strategy is to select the entry $a_{ij}^{(k)}$, from the $(n-k) \times (n-k)$ sub matrix that minimises the expression $(r_i^{(k)} - 1)(c_j^{(k)} - 1)$, where r_i is the number of non zeros in row i and c_j is the number of non zeros in column j .

One way to interpret this strategy is to say that it chooses the pivot which modifies the least coefficients in the remaining sub matrix at each elimination step.

Here we present a 'Block Markowitz' strategy for the case where A can be partitioned into a block form with the blocks A_{ij} exhibiting a structured sparsity pattern.

The algorithms exploit the structural form of the blocks and they are particularly tailored for use with pivot blocks which are diagonal, bidiagonal, tridiagonal or general forms of these structures.

IMPLICIT NEWTON'S METHOD IN THE UPDATE OF MATRIX FACTORIZATIONS

Marek Szularcz (Kingston University) & **Svetlana Lyle** (Kingston University).

We present an alternative zero-finder for an important class of secular equations arising in the update of symmetric eigensystems and SVD. The method has been developed in connection with the update of the spectral decomposition of the matrix appearing in a quadratic objective function, subject among other constraints, to a set of linear inequalities. We found that each branch of the curve of the secular equation can be transformed to such a form that the ordinary Newton's method can be safely applied, giving certain advantages over the standard technique. The transformation mentioned here can be controlled in such a way that the resulting function can be made either concave or convex, allowing us to choose a better, more 'linear' option. We present some numerical examples computed on a Convex C3840.

ON SINGULAR INTEGRO-DIFFERENTIAL EQUATIONS

Ezio Venturino (Università di Catania, Italy)

In this talk we want to consider integro-differential equations containing a Cauchy principal value integral, formulated over the compact interval $[-1, 1]$. We suitably modify earlier proposed elementary low order schemes for the calculation of singular integrals in order to apply them to the solution of singular integral equations. We finally couple them with standard methods for the solution of differential equations in order to solve the problem. The purpose of the study is the attempt of an error analysis that, to our knowledge, is still lacking for such equations; this in spite of the considerable literature in the field developed in the past twenty five years.

AN ASYMPTOTIC EXPANSION FOR INTEGRATION OVER A DISK

P. Verlinden (Katholieke Universiteit Leuven, Belgium)

The paper deals with the numerical evaluation of the integral over a disk

$$\int_0^1 r^{1+\alpha} \int_0^{2\pi} f(r \cos t, r \sin t) dt dr.$$

Compound integration rules are obtained by a subdivision of the integration region into a subdisk and a collection of curved rectangles, whereby the integral over the subdisk is approximated with a cubature formula Q_2 and the integral over each curved rectangle is approximated with a nonlinearly scaled cubature formula Q_1 for a rectangle.

It is shown that subdividing the integration region corresponds to applying a linear averaging operator to the integrand. The asymptotic behaviour of the iterates of this operator follows from its spectral analysis. The obtained asymptotic error expansion allows the use of extrapolation as in Romberg integration.

A SHADOWING LEMMA APPROACH TO GLOBAL ERROR ANALYSIS FOR INITIAL VALUE ODES

Erik S. Van Vleck (Simon Fraser University, Canada)

We show that for dynamical systems that possess a type of piecewise hyperbolicity in which there is a nondecrease in the number of stable modes the global error in a numerical approximation may be obtained as a reasonable magnification of the local error. In particular, under certain conditions we prove the existence of a trajectory of the given ordinary differential equation uniformly close to a given numerically computed orbit of the same differential equation by allowing for different initial conditions. Two approaches for numerically obtaining a posteriori bounds on the global error are presented and are applied to the logistic equation, the forced pendulum equation and the space discretized Chafee-Infante equation.

APPROXIMATIONS TO SHALLOW WATER FLOWS USING VARIATIONAL PRINCIPLES

S. L. Wakelin (University of Reading)

Hamilton's principle is used to create a variational principle which has as its natural conditions the equations of irrotational motion in an incompressible homogeneous fluid with a free surface. By applying the shallow water approximation this reduces to a given a variational principle for shallow water flow.

Finite element approximations to channel flows can be obtained using the variational principle. Examples are given for continuous and discontinuous solutions of the shallow water equations.

PACKAGE PARASPAR FOR GENERAL SPARSE MATRICES

Jerzy Waśniewski (Technical University of Denmark)

Package PARASPAR is a set of FORTRAN subroutines for solving linear systems of algebraic equations

$$Ax = b$$

whose coefficient matrices are assumed to be (i) real, (ii) large and (iii) general sparse. It is not assumed that the matrix has any special property (such as symmetry or positive definiteness) or any special pattern (such as bandedness).

The subroutines of the package PARASPAR are optimized for parallel computers with shared memory and with not too many tightly connected processors. In fact the subroutines were extensively tested on FX/80, FX/2800 ALLIANTS and CONVEX parallel computers, but the most important processes that can be carried out in parallel are well-separated (in subroutines that can be called concurrently in loops). Therefore it is easy to optimize the package on other computers.

At the end of the factorization step the use of sparse matrix technique becomes less efficient. Therefore it is more profitable to switch to the dense matrix technique at the

end of the computations if the active submatrix becomes sufficiently dense. Switching to dense matrix technique is available in all options for solving systems of linear algebraic equations that are currently available in the package PARASPAR.

New non-zero elements (fill-ins) are created in the course of computations on the places where the original elements of the matrix were zeros. Often such elements are in some sense small. Therefore it is profitable to remove all small elements that are created during the computations. The factors L and U so calculated are usually very sparse and they are obtained cheaply. On the other hand, they may be inaccurate (because of dropping some elements) and they cannot be used to calculate the solution directly. However the factors L and U calculated by dropping small elements can be used as preconditioners in iterative methods. Two preconditioned iterative methods are currently used in package PARASPAR: (i) a simple iterative refinement and (ii) an ORTHOMIN algorithm.

The ORTHOMIN algorithm can also be used as a pure iterative method. This option in package PARASPAR is normally not very efficient (for general matrices the iterative methods are normally not convergent), but for some matrices it may be the best choice.

SOLVING GENERALIZATIONS OF ORTHOGONAL PROCRUSTES PROBLEMS

G A Watson (University of Dundee)

The orthogonal Procrustes problem involves finding an orthogonal matrix which transforms one given matrix into another in the least squares sense: thus it requires the minimization of the Frobenius matrix norm. We consider the solution of this problem for some other orthogonally invariant norms.

APPROXIMATE GREENS FUNCTION PRECONDITIONING FOR THE SEMICONDUCTOR DEVICE EQUATIONS

Andy Wathen (University of Bristol) & *Steve Chandler* (University of Bristol).

The 'Drift-diffusion model' for semiconductor devices comprises three coupled partial differential equations for an electric potential, and concentrations of negatively and positively charged particles. One equation is a self-adjoint Poisson type equation with nonlinear source terms whilst the other two 'current continuity' equations are of nonlinear convection diffusion type. Common numerical methods for their solution involve a successive iteration ('Gummel iteration') followed by Newton's method. In each phase of the solution process large linearised systems of equations require to be solved. Non-symmetric Krylov-subspace iterative methods such as the recent BiCGSTAB method of Van der Vorst are popular for these systems.

We will describe two ideas for enhancing the convergence of such linear iterative solvers by employing approximate Greens Functions. The first, involving the incorporation of the effect of inhomogeneous boundary conditions into the initial iterate, is inexpensive to compute and has been seen to reduce the number of iterations required for convergence in computations. The second involves using a preconditioner constructed from an approximate Greens function.

We will present computational results showing the performance of these techniques on practical semiconductor problems taken from the Philips 'TESSA' device simulation programme. These techniques are more generally applicable and may be advantageous in other partial differential equation boundary value problems.

COMPUTATION OF HOPF BIFURCATION WITH BORDERED MATRICES

Bodo Werner (University of Hamburg, Germany)

Bordered matrices and linear systems with bordered coefficient matrices are of interest in numerical steady state bifurcations.

We will be concerned here with bordered linear systems

$$\begin{pmatrix} A^2 + \nu I & Ar & r \\ l^T A & 0 & 0 \\ l^T & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0_n \\ 1 \\ 0 \end{pmatrix},$$

with $l, r \in \mathbb{R}^n$. This linear system is closely related to Hopf bifurcation of $x' = f(x, \lambda)$, setting $A := f_x(x, \lambda)$ and requiring two scalar equations $\alpha = \alpha(A, \nu) = 0$ and $\beta = \beta(A, \nu) = 0$. Then $\nu = \omega^2$ is the *Hopf number* associated with the Hopf frequency ω of the eigenvalues $\pm i\omega \in \sigma(A)$ of the *Hopf matrix* A .

The system can be derived from the extended Hopf system in Werner-Janovsky 1991—a modification of that in Roose-Hlavacek 1985 allowing $\nu \leq 0$ and hence including *imaginary Hopf points*.

A *test function* for Hopf points in the sense of Werner 1992 is constructed by nonlinear scalar elimination of the Hopf number ν . A relation to a certain generalized eigenvalue problem $(P - \nu Q)x = 0$ of a matrix pencil with singular Q is established.

It is shown that numerical Hopf bifurcation (detection and computation of Hopf points, computation of Hopf curves) can be based on bordered systems. Formulas are given for the derivatives of α and β (and of the corresponding test function) as functions of A (or x, λ) and ν which can be cheaply evaluated.

Numerical examples are given.

ODES WITH SINGULAR POINTS AND SINGULAR COLLOCATION MATRICES

K. Wright (University of Newcastle-upon-Tyne)

For differential equations of the form

$$y' = A(t)y + b(t)$$

with initial conditions, solution by collocation (or equivalently IRK) methods produces a set of simultaneous linear equations at each step. These equations can be singular but this will not happen for sufficiently small interval size if A is bounded. However, this is not necessarily true if a singular point is present even when there is a well behaved solution to the differential equation, and the singular point is not one of the collocation points. Examples will be given which demonstrate this both for linear equations and the linearized form of non-linear equations.

Implications for integrating through singular points will be considered, along with an application to systems derived to solve the analytic singular value decomposition problem, which was the motivation for this work.

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Additional Abstracts

Invited:

MULTI-RESOLUTION METHODS IN NUMERICAL ANALYSIS

R. Temam (Université Paris Sud, France)

Parallel and large scale computing allow the utilization of large numbers of unknowns. The handling of such large numbers of unknowns leads to new problems in numerical analysis: data compression, differentiated treatment of short and long waves, etc. In this lecture we shall discuss new algorithms addressing this problem, the Nonlinear Galerkin Method and the Incremental Unknown Method.

Submitted:

NUMERICAL SOLUTIONS OF HAMILTONIAN SYSTEMS

G. Ramaswami (University of Cambridge)

It is known that many Runge-Kutta-Nyström methods can be derived by collocation. In this talk we prove that the only s -stage symplectic Runge-Kutta-Nyström method that can be obtained by ordinary collocation is of order $2s$ and implicit. We also extend the idea of perturbed collocation to Runge-Kutta-Nyström methods and derive symplectic Runge-Kutta-Nyström methods using this technique. We obtain symplectic implicit s -stage Runge-Kutta-Nyström methods of order $2s - 1$ and $2s - 2$.

MULTIPLICATIVE SCHWARTZ FACTORIZATION FOR PRECONDITIONING RESERVOIR SIMULATION APPLICATIONS

J. C. Díaz (University of Tulsa, USA) *L. Chu, M. Komara & A. C. Reynolds* (University of Tulsa, USA)

We discuss a multiplicative Schwartz incomplete factorization for local grid refinement in a heterogeneous reservoir simulation application. Peaceman's wellbore formulation is used to model the well terms. The results illustrate how the local grid refinement with incomplete Schwartz preconditioning is able to accurately predict the wellbore reservoir pressure response in a system under a variety of production conditions.