

17th Biennial Conference
on
Numerical Analysis

24 June—27 June, 1997

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Introduction

Welcome to Dundee! We hope that your stay will be an enjoyable one and ask you please to note the following.

1. General

There will be an information/registration desk in the foyer of the Tower Building throughout the conference.

2. Accommodation

Breakfast in Belmont Hall is available from 7.45 to 8.45, lunch is served at 12.50 (13:10 on Friday) and dinner at 18.30 (except Thursday).

3. Lecture Rooms

In the timetable, **L/T** refers to the main Lecture Theatre on the ground floor of the Tower Building, behind the reception desk.

Lecture room **T4** is on the first floor of the Tower Building, **T9** is on the second floor. Both are easily reached by the main staircase to the left of the lifts.

The room labelled **G9–11** is situated at the rear of the main Lecture Theatre. It may be accessed from either side, or through the rear, of the main Lecture Theatre.

4. Session Chairs

It is hoped that those who are listed as chairing the various sessions will be willing to assist in this way. Time has been allowed in the program for participants to change lecture rooms where appropriate, and chairs are asked to keep speakers strictly to the timetable.

5. Coffee and Tea Breaks

Morning coffee and afternoon tea will be provided in Bonar Hall: turn right out of the back door of the Tower, right again and Bonar Hall is on the left.

6. Bar Facilities

A bar is provided in Belmont Hall for all participants. It will be open during the times 18.00–23.00 on the nights of Monday to Wednesday.

A selection of canned drinks will also be available for purchase at Lunchtime.

7. Conference Reception

The University of Dundee will give a reception for all participants in the TV lounge in Belmont Hall from 20.00 to 22.00 on Tuesday 24 June.

8. Conference Dinner

The conference dinner will be held in Belmont Hall on Thursday 26 June at 20.00, and sherry will be provided beforehand from 19.30. The guest speaker will be Dr George Phillips, University of St Andrews.

Invited Speakers

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Abstracts of Invited Talks

ADAPTIVE FINITE ELEMENTS AND COLLIDING BLACK HOLES

D N Arnold, A Mukherjee & L Pouly (*Pennsylvania State University, Department of Mathematics, 228 McAllister Building, University Park, Pennsylvania 16802-6403, USA*)

According to the theory of general relativity, the relative acceleration of masses generates gravitational radiation. Although gravitational radiation has not yet been detected, it is believed that extremely violent cosmic events, such as the collision of black holes, should generate gravity waves of sufficient amplitude to detect on earth. The massive Laser Interferometer Gravitational-Wave Observatory, or LIGO, is now being constructed to detect gravity waves. Consequently there is great interest in the computer simulation of black hole collisions and similar events, based on the numerical solution of the Einstein field equations. This talk will introduce the scientific, mathematical, and computational problems and discuss the development of a computer code to solve the initial data problem for colliding black holes, a nonlinear elliptic boundary value problem posed in an unbounded three dimensional domain which is a key step in solving the full field equations. The code is based on finite elements, adaptive meshes, and a multigrid solution process and the talk will particularly emphasize the mathematical and algorithmic issues arising in the generation of adaptive tetrahedral meshes.

SYMMETRY BASED NUMERICAL METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

C J Budd (*University of Bath, School of Mathematical Sciences, Bath, UK*)

It has long been recognised that many important partial differential equations arising in mathematical physics and applied mathematics are invariant to a Lie group of transformations and that by exploiting this invariance exact solutions can be determined in many cases. Remarkably such solutions are often also global attractors for more general solutions of the equations given a variety of initial data. Symmetry also plays an important role in studies of ordinary differential equations describing the evolution of systems on manifolds. When such equations are discretised using a numerical method, the symmetry properties are often lost and the resulting discrete solutions fail to capture important qualitative features of the underlying differential equation. Recently, however, there has been much progress in developing numerical methods for both partial and ordinary differential equations which inherit the symmetry properties of the underlying system. Such methods afford the promise of capturing important qualitative information about the underlying differential equation over long time periods.

This talk will give a review of some of the latest developments in the study and application of numerical methods based upon symmetry considerations, looking at results from several different workers in the area. It will start by studying numerical methods for ordinary differential equations, demonstrating that group based methods lead to discretisations which differ from those obtained from the usual Taylor series expansion approach and which have excellent convergence properties over very long time intervals. We will then look at methods for partial differential equations. The key idea here is a synthesis of the ordinary differential equation approach with the use of a spatially adapted (and dynamic) mesh. Here the motion of the mesh is determined by the group either directly or by using an approach based upon equidistribution. Such methods have good qualitative

dynamics and the use of symmetry gives also offer a means of analysing their convergence properties (traditionally a difficult task for an adaptive method). We will look at a variety of examples including problems with nonlinear diffusion, integrable systems and partial differential equations which have solutions that become singular in a finite time. Using results of computations on these problems we will discuss both the advantages, disadvantages and generality of using symmetry based methods.

AN ADAPTIVE AND PARALLEL FRAMEWORK FOR PARTIAL DIFFERENTIAL EQUATIONS
J E Flaherty (*Rensselaer Polytechnic Institute, Department of Computer Science, Troy, NY 12180, USA*)

Adaptive computational techniques are having a dramatic impact on the way that scientists and engineers solve problems involving partial differential equations. Like adaptivity, parallel computation is being used to an increasing degree. We are developing a framework for adaptive and parallel computation that is capable of (i) generating three-dimensional unstructured meshes of tetrahedral elements, (ii) automatically refining and coarsening these meshes, (iii) partitioning the computation into subdomains that may be processed in parallel, and (iv) maintaining a balanced parallel computation through element migration. Mesh generation is supported by a hierarchical database in which spatial regions are linked to their bounding faces, which are linked to their bounding edges, which are linked to their endpoints. The database is connected to geometrical modeling procedures and to a parallel library having capabilities for processor scheduling and reassignment. The adaptive finite element framework is being used to study several flow problems. Transient problems may be solved by local refinement methods which have spatially-dependent time steps.

BLOCK TRIANGULAR ORDERINGS AND FACTORS FOR SPARSE MATRICES IN LP

R Fletcher (*University of Dundee, Department of Mathematics and Computer Science, Dundee, DD1 4HN, UK*)

Tarjan's algorithm together with depth-first transversal search is an efficient method for finding an irreducible block triangular ordering of a nonsingular sparse matrix A . However, when used in conjunction with $PA = LU$ factors within the blocks, there are difficulties in finding a simple data structure which permits linear systems involving A or A^T to be solved efficiently. Thus many sparse matrix codes ignore the possibility of using block orderings. The possibility of using the less well known technique of Implicit LU factors is considered and it is shown that a much more simple data structure is available. For certain irreducible sparse matrix patterns the fill-in with this technique is no worse than that incurred by LU factors.

In Linear Programming the invertible representation of the basis matrix must also be updated when one column in A is replaced by another, and this causes more problems for an algorithm based on block factors. It is shown how the block ordering can be updated efficiently when the basis is changed. Some information in the Implicit LU factors is unaffected by the update. How best to deal with the part that is affected is currently under review.

This work is ongoing and current progress will be reported at the conference.

USING NONORTHOGONAL LANCZOS VECTORS IN THE COMPUTATION OF MATRIX FUNCTIONS

A Greenbaum, V Druskin & L Knizhnerman (*New York University, Department of Computer Science, Courant Institute, 251 Mercer Street, New York, NY 10012, USA*)

The symmetric Lanczos algorithm uses a three-term recurrence to construct an orthonormal basis for the Krylov space corresponding to a symmetric matrix A and a nonzero starting vector b . These basis vectors can be used for a number of purposes including solving linear systems $Ax = b$ and computing the matrix exponential $\exp(-tA)b$. Unfortunately, the basis vectors produced in finite precision arithmetic are not orthogonal — they may even be linearly dependent. We show why the computed basis vectors can still be used effectively for these purposes.

For nonsymmetric problems, the basis vectors produced by the Lanczos algorithm are not orthogonal even in exact arithmetic. (They are biorthogonal.) One might expect some of the same proof techniques to be relevant to this case. We discuss the interesting open problem of deriving error bounds for nonsymmetric Lanczos-based linear system solvers such as BiCG and QMR. In particular, the role of the left starting vector is analyzed.

ORDER BARRIERS FOR SYMPLECTIC MULTI-VALUE METHODS

E Hairer & P Leone (*University of Geneva, Section de Mathématiques, CH-1211 Genève 24, Switzerland*)

For the numerical solution of ordinary differential equations, multi-value methods advance the approximate solution in a higher dimensional space. We show that this mapping possesses an invariant manifold, on which the multi-value method is equivalent to a one-step method. Assuming this underlying one-step method to be symplectic, we prove that the order of the multi-value method has to be at least twice its stage order. As special cases of this result we obtain: multistep methods can never be symplectic; the only symplectic one-leg method is the implicit mid-point rule, and the Gauss methods are the only symplectic Runge-Kutta collocation methods.

STABILITY OF HOUSEHOLDER QR FACTORIZATION FOR WEIGHTED LEAST SQUARES PROBLEMS

N J Higham & A J Cox (*University of Manchester, Department of Mathematics, Manchester, M13 9PL, UK*)

For least squares problems in which the rows of the coefficient matrix vary widely in norm, Householder QR factorization (without pivoting) has unsatisfactory backward stability properties. Powell and Reid showed in 1969 that the use of both row and column pivoting leads to a desirable row-wise backward error result. We give a reworked backward error analysis in modern notation and prove two new results. First, sorting the rows by decreasing ∞ -norm at the start of the factorization obviates the need for row pivoting. Second, row-wise backward stability is obtained for only one of the two possible choices of sign in the Householder vector.

FINITE VOLUME SCHEMES IN MULTIDIMENSIONS: THEORY AND APPLICATIONS

D Kröner (*University of Freiburg, Institut fuer Angewandte Mathematik, Hermann-Herder-Str.10, 79104 FREIBURG, Germany*)

For the discretization of the Euler or the compressible or incompressible Navier-Stokes equations with large Reynolds numbers it is necessary to introduce numerical damping in order to get stable schemes. In a quite natural form this is established by upwind

discretizations of first or higher order. The distinction between first and higher order upwind methods in the context of finite volume or finite difference methods (e.g. MUSCL methods) is still not rigorous and usually based on the analysis of the truncation error which is meaningless for nonlinear problems and also for linear problems on unstructured grids. A useful criterion can only be given by a priori error estimates of the form $\|u - u_h\| \leq Ch^\alpha$ (u : exact solution, u_h : numerical solution) with different α for first and higher order schemes respectively. Unfortunately these estimates are not available for the most interesting problems even not for the simple nonlinear scalar conservation laws in 2-D. For first order finite volume schemes on unstructured grids applied to nonlinear problems, error estimates with $\alpha = \frac{1}{4}$ and for the streamline diffusion shock capturing method applied to the linear transport equation with $\alpha = \frac{3}{2}$ are known already. Numerical experiments for upwind finite volume methods indicate that one should also expect in this case $\alpha = 2$ for smooth solutions. But theoretically justified error estimates for upwind finite volume schemes of higher order, which also indicate the higher order, are still an open problem. The convergence has been proved by a series of papers but the theoretical order of convergence has not been established up to now. Since it is too hard to prove this directly for conservation laws, we have applied the upwind finite volume schemes of higher order to the singular perturbed linear elliptic convection dominated diffusion equation in multidimensions in order to get these estimates. These results have been confirmed by numerical experiments. Furthermore we shall report on the application of finite volume schemes to different numerical applications in 3-D.

INTERIOR POINT METHODS VS SEQUENTIAL QUADRATIC PROGRAMMING FOR NONLINEAR OPTIMIZATION

J Nocedal (*Northwestern University, Dept of Elec Eng and Computer Science, Evanston, Illinois 60208-0001, USA*)

Interior point methods are emerging as an important approach for solving large nonlinear optimization problems with inequality and equality constraints. We discuss how these interior point methods must differ from their linear counterparts in order to be robust and efficient. We also show that the ill-conditioning in the step computation can be handled quite well by a new algorithm based on trust region techniques. We compare the strengths of this approach with those of Sequential Quadratic Programming methods, and present numerical tests illustrating their relative performance. We conclude with the description of a new preconditioning technique for the conjugate gradient iteration used in the step computation of our new interior point method.

TRUST REGION CALCULATIONS REVISITED

M J D Powell (*University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK*)

Trust region changes to the variables in many trust region algorithms for optimization calculations are derived from the following problem. Minimize a quadratic function $Q(\underline{d})$, $\underline{d} \in \mathcal{R}^n$, subject to $\|\underline{d}\| \leq \Delta$, where Q and $\Delta \in \mathcal{R}$ are given and where the vector norm is Euclidean. Because the required $\underline{d}$ is a stationary point of the Lagrange function $Q(\underline{d}) + \frac{1}{2}\lambda(\|\underline{d}\|^2 - \Delta^2)$, $\underline{d} \in \mathcal{R}^n$, for some $\lambda \geq 0$, it satisfies the linear system of equations $(G + \lambda I)\underline{d} = -\underline{g}$, where $G = \nabla^2 Q$ and $\underline{g} = \nabla Q(0)$. This system may be solved for many trial values of λ , but $\mathcal{O}(n^3)$ operations are required for each λ if G is a general $n \times n$ symmetric matrix that has no useful sparsity. In optimization algorithms, however, when second derivatives are not

available explicitly, each G is usually formed by making a rank one or rank two update to the G of the previous iteration, and then work can be saved for $n \geq 40$ by applying an orthogonal similarity transformation to G that yields a symmetric matrix of band width about $n^{2/3}$. This technique will be described and discussed briefly. It increases the usefulness of the methods for adjusting λ that were developed about 20 years ago. Therefore that work will be reviewed. A specific procedure of that kind for calculating $\underline{d}$ to prescribed accuracy will be recommended. Its main features will be demonstrated by some numerical results.

LONG-TIME STEP METHODS FOR OSCILLATORY DIFFERENTIAL EQUATIONS

J M Sanz-Serna, B García-Archilla & R D Skeel (*Universidad de Valladolid, Departamento de Matematica Aplicada y Computacion, Valladolid, Spain*)

We consider numerical integration schemes for nondissipative dynamical systems in which multiple time-scales are present. We were motivated by problems in molecular dynamics, where, for instance, the vibrational frequencies of individual chemical bonds are much higher than the frequencies associated with the large-scale bending of the (macro-)molecule under study. It is assumed that one can do an explicit separation of the forces in the problem into fast forces and slow forces such that (i) the fast forces contain all the high frequency part of the solution, (ii) the fast forces are conservative and (iii) the reduced problem consisting only of the fast forces can be integrated much more cheaply than the full problem. The fast forces are allowed to have low frequency components. We study algorithms that employ samples of the slow forces and also make use of the possibility of solving the reduced problem. It is assumed that the overall cost of such an algorithm is primarily determined by the number of samples of the slow forces. Two examples follow.

In a macromolecule with N atoms, there are $O(N)$ forces associated with the chemical bonds along the molecule and these cause the high frequency motion; other interactions such as electrostatic or van der Waals forces possess a higher $O(N^2)$ complexity as they involve all pairs of atoms but lead to slower motions. Here the reduced problem only includes the $O(N)$ forces in the chemical bonds and its solution may be considered to have a negligible cost.

When solving a nonlinear wave equation $u_{tt} = u_{xx} + F(u, u_x)$ the reduced problem $u_{tt} = u_{xx}$ can be solved virtually exactly from t to $t + \Delta t$ by means of a spectral method. The cost of a spectral step in the reduced problem is independent of Δt and therefore the cost of an algorithm is determined by how often it requires to sample the softer term $F(u, u_x)$.

A long-time step method is one in which the step size exceeds half the period of the fastest mode present in the full system. An obvious candidate to the role of long-time step method is a simple splitting scheme (sometimes called the impulse method) where the numerical solution is advanced from t to $t + \Delta t$ by integrating the reduced problem and then the slow forces are used to increment the momenta at $t + \Delta t$. We show that both the accuracy and the stability of the impulse method are poor. An alternative "mollified" method is suggested and analyzed.

THE SEARCH FOR A GOOD BASIS

G Strang (*Massachusetts Institute of Technology, Department of Mathematics, USA*)

An image corresponds to a very long vector, with one component for each pixel (three

components for a color image). By a change of basis the long vector is concentrated into a much smaller number of components, ready for compression. We study the block Toeplitz matrix that produces a new basis from a bank of two filters – lowpass and highpass. The filter coefficients determine the success of the compression. They also determine whether iteration of the lowpass filter (with rescaling) will lead to a useful wavelet basis for function spaces.

Thus the construction of wavelets comes from a problem in matrix analysis. Actual compression uses 4-5 iterations of the basis change.

EIGENVALUES AND CARD SHUFFLING – THE ‘CUTOFF PHENOMENON’ IN MARKOV CHAINS

Ll. N Trefethen (*Cornell University, Dept. of Computer Science, Ithaca, NY 14853, USA*)

Diaconis and others have shown that certain Markov chains – a celebrated example involves shuffling a deck of cards – exhibit a sharp “cutoff phenomenon” in which, after an initial period of seemingly little progress, convergence to the steady state occurs quite suddenly. In these examples, the transient behavior of the powers of a matrix differs strikingly from the asymptotic behavior governed by the second eigenvalue. How can this be? Is it an artifact of using the 1-norm instead of the 2-norm? Is it caused by the non-normality of the matrix? We examine one of the standard examples of these problems, random walk on a hypercube (closely related to the Ehrenfest urns), and find there are some surprises.

THE CONVERGENCE OF ITERATIVE SOLUTION METHODS FOR SYMMETRIC AND INDEFINITE LINEAR SYSTEMS

A Wathen, B Fischer & D Silvester (*Oxford University, Computing Laboratory, Oxford OX1 3QD, UK*)

Real symmetric and indefinite matrices arise in various contexts in the numerical solution of partial differential equations as well as in other areas of Numerical Analysis, notably optimisation. For large sparse linear systems iterative methods such as the MINRES and SYMMLQ methods of Paige and Saunders can be attractive, particularly when rapid convergence can be guaranteed.

We will present a descriptive analysis of the convergence of the Minimum Residual method in its application to discrete saddle-point problems arising in partial differential equations.

Abstracts of Contributed Talks

ASYMPTOTIC GLOBAL ERROR ESTIMATION FOR VARIABLE STEP-SIZE AND ONE-STEP METHODS

R Aïd (*EDF-DER-FCR, 1, Avenue du Général de Gaulle F-92141 Clamart Cedex and LMC-IMAG, 51, Rue des Mathématiques, BP 53, F-38 041 Grenoble Cedex 9, France*)

It is usual in the case of variable step-size integration for one-step methods to be satisfied with the first term of the asymptotic expansion of the global error [3]. However, the proof of the convergence of Zadunaisky's technique as well as Solving for the Correction in the case of constant step-size makes use of more than one term of this expansion. Recently, Calvo et al. [1] gave a proof for the convergence of these two techniques in the case of an XEPS control using a one-term asymptotic expansion of the global error together with the special structure of the local errors for these techniques [2].

The aim of this talk is to provide another analysis of these two techniques in the case of variable step-size for one-step methods. Relaxing the hypothesis on the local error control and restricting ourselves to the case of *theoretical* local error control, i.e. the step-size is supposed to be the largest such that the norm of the local error estimate is lower than the absolute tolerance, it is shown that the global error admits a similar asymptotic expansion w.r.t. the tolerance as in the case of constant step-size integration. The convergence of Zadunaisky's technique follows immediately.

Moreover, the special Dormand and Prince's r -terms estimation formulae are shown to exhibit a valid order of convergence w.r.t. the maximum step-size for any convergent grid sequence.

Finally, the case of Solving for the Correction technique is discussed. Usually, it is assumed that this technique needs a secondary integration with a method at least as precise as the first one. It is shown here that this condition is not necessary. Moreover, the case of other types of interpolation process than classical Lagrangian interpolation of the numerical solution are considered.

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[2] J. R. Dormand, M. A. Lockyer, N. E. McGorrigan, and P. J. Prince. Global error estimation with Runge-Kutta triples. *Computers Math. Applic.*, 18(9):835–846, 1989.

[3] D. J. Higham. Global error versus tolerance for explicit Runge-Kutta methods. *IMA J. Numer. Anal.*, 11:457–480, 1991.

HYPERBOLIC PROBLEMS WITH SOURCE TERMS, PART II: MACCORMACK TYPE METHODS

M A Aves, D F Griffiths & D J Higham (*University of Dundee, Department of Mathematics and Computer Science, Dundee DD1 4HN, UK*)

MacCormack's method is widely used in the solution of hyperbolic systems. We show that in the presence of source terms, the conventional implementation is not stable for Courant numbers close to one unless a small time-step is used. A simple modification is introduced to remove this defect. We also show how the modification affects spurious behaviour with nonlinear source terms.

FINDING INTERVALS CONTAINING OPTIMAL VALUES OF PARAMETERS OF THE ASOR METHOD

E Babolian & M T Darvishi (*Tehran Institute of Mathematics, 599, Taleghani Ave., Tehran, Iran*)

The accelerated Over-Relaxation method, called AOR or ASOR, is a generalization of the SOR method. This method has two parameters r, w ; considering systems with special coefficient matrices, sufficient conditions of the values of r and w have been obtained to guarantee its convergence. Obtaining optimal values of r and w is the most difficult part of the method. Considering systems with special row diagonally dominant matrices we determine small intervals containing optimal values of r and w . We define the function $g(r, w)$, which is the upper bound of the spectral radius of iteration matrix and obtain its minimum. Using computer we show that optimal values of r and w belong to a small neighborhood of r and w which minimize $g(r, w)$. To enhance the theory, numerical examples are presented.

LEAST SQUARES, EQUIDISTRIBUTION AND CONSERVATION

M J Baines (*University of Reading, Department of Mathematics, PO BOX No 220, Reading RG6 2AX, Berks, UK*)

It is shown that, for a vector valued function F which is piecewise conforming on a partition of a region V with a prescribed flux across the boundary dV , minimisation of the l_2 norm of the fluctuation of F over the internal nodes of the partition (with the nodes free to move) is equivalent to minimisation of the l_2 norm of the differences in the fluctuations of F over all the elements of the partition. In this sense l_2 minimisation is equivalent to a measure of equidistribution.

If $F = Ua$ where U is a piecewise linear function on a triangular partition of a polygonal region P and a is divergence free and if U is prescribed on dP , the result is also true for the l_2 norm of $a \cdot \text{grad}U$ weighted by the areas of the elements.

Applications in one and two dimensions are discussed although the results hold in any number of dimensions.

WHAT DOES IT MEAN FOR A HERMITIAN EIGENVALUE PROBLEM TO BE WELL-BEHAVED?

J L Barlow & I Slapnicar (*The Pennsylvania State University, Computer Science and Engineering Department, University Park, PA 16802, USA*)

In recent years, significant progress has been made in understanding how to solve eigenvalue problems more accurately. We give a perturbation theory that includes much of this progress. The main application of this work is the development of robust software for eigenvalue problems. The efforts described here have had great influence on the eigenvalue codes in the LAPACK project.

There are two important thrusts to these efforts. The first is to find classes of matrices which are “well behaved.” These are matrices for which structured relative changes in the entries of the matrices cause only relative changes in the eigenvalues. We also expect that the invariant subspaces associated with clusters of eigenvalues will be very stable. The second thrust is to find algorithms that compute the eigenvalues and eigenvectors to the expected accuracy. This talk will define a well-behaved matrix discuss its characterization.

The research of Jesse L. Barlow was supported by the National Science Foundation under grant no. CCR-9424435.

THE ADAPTIVE SOLUTION OF SELF-ADJOINT BOUNDARY VALUE PROBLEMS USING A POSTERIORI ERROR ESTIMATES AND GRID EQUIDISTRIBUTION

G Beckett & J A Mackenzie (*University of Strathclyde, Department of Mathematics, Glasgow G1 1XH, UK*)

In this talk we consider the adaptive numerical solution of self-adjoint boundary value problems using finite element methods. We first review the derivation of a posteriori estimates of the energy norm of the error. These are based on norms of a local projection of the error. We discuss the practical evaluation of this projected error by solving a series of local problems. These error estimates are then used to define a monitor function which is equidistributed over the domain. The overall algorithm aims to drive the error below a given tolerance using a combination of enrichment (h-refinement) and mesh movement (r-refinement), and is shown to give efficient quantitative control of the error for a number of test cases, including singularly perturbed problems.

ON THE ACCURACY OF RADIAL BASIS FUNCTION INTERPOLATION ON FINITE UNIFORM GRIDS

A Bejancu (*University of Cambridge, DAMTP, Cambridge, UK*)

Let m be a nonnegative integer and let $\{\phi(t^{1/2}) : 0 \leq t < \infty\}$ be a continuous function that is conditionally strictly positive definite of order m . For each positive integer n , let $h = n^{-1}$ and let $\{x_j : j = 1, 2, \dots, (n+1)^d\}$ be the vertices of the uniform grid of mesh-size h on the unit d -dimensional cube $[0, 1]^d$. Given $f : [0, 1]^d \rightarrow \mathbf{R}$, we consider the unique radial basis function (RBF) s_h of the form

$$s_h(x) = \sum_{j=1}^{(n+1)^d} c_j \phi(\|x - x_j\|) + p_h(x)$$

that satisfies the interpolation conditions $s_h(x_i) = f(x_i)$, $i = 1, 2, \dots, (n+1)^d$, where $p_h \in \mathcal{P}_{m-1}(\mathbf{R}^d)$, $\|\cdot\|$ denotes the Euclidean norm on $\mathbf{R}^d$ and the coefficients $\{c_j : j = 1, 2, \dots, (n+1)^d\}$ are subject to the constraints

$$(1) \quad \sum_{j=1}^{(n+1)^d} c_j p(x_j) = 0, \quad \forall p \in \mathcal{P}_{m-1}(\mathbf{R}^d).$$

For a large class of basis functions ϕ , we show that the uniform norm of the error $f - s_h$ on a compact subset K of the interior of $[0, 1]^d$ enjoys the same rate of convergence to zero as the error of RBF interpolation on the infinite uniform grid $h\mathbf{Z}^d$, provided that f is sufficiently smooth. As an example, if $\phi(t) = t^2 \ln t$ (so $m = 2$), then $\|f - s_h\|_{\infty, K} = \mathcal{O}(h^{d+2})$. For this choice of ϕ and for $d = 1$, numerical tests illustrate the above result and the fact that loss of accuracy occurs near the two endpoints of $[0, 1]$. We also discuss the replacement of (1) by other types of constraints that give improved uniform convergence on $[0, 1]$ in practice.

EXTENDING LSQR TO GENERALISED LEAST-SQUARES AND SCHUR COMPLEMENT PROBLEMS WITHOUT RESORTING TO CHOLESKY DECOMPOSITIONS

S Benbow (*University of Bath, School of Mathematics, Bath BA2 7AY, UK*)

Linear systems of the form

$$\begin{bmatrix} A & B \\ B^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix},$$

where the $n \times n$ symmetric positive-definite matrix A and the $n \times m$ full column rank matrix B ($n \geq m$) are large and sparse, can arise in the numerical solution of many problems in applied mathematics including optimisation, computational fluid dynamics and electrical network simulation. These systems can be viewed as generalised least-squares problems with respect to an appropriate norm, and this talk describes a new iterative method of solution which exploits the least-squares nature of the problem. The method, LSQR(A^{-1}), is shown to be a natural extension of the LSQR algorithm of Paige and Saunders, with generalised orthogonality properties so that the Cholesky factor of A is not required. Instead it is only assumed that some method of calculating the effect of A^{-1} on a vector is available.

Numerical experiments comparing LSQR(A^{-1}) with similar preconditioned Krylov methods are described which demonstrate that LSQR(A^{-1}) exhibits superior numerical properties when the Schur complement matrix, $B^T A^{-1} B$, is ill-conditioned.

REGULARISED SOLUTION OF FREDHOLM INTEGRAL EQUATIONS OF THE FIRST KIND HAVING SYMMETRIC L_2 KERNEL

R P Bennell (*Cranfield University (RMCS), Department of Applied Mathematics and OR, Shrivenham, SN6 8LA, UK*)

We consider regularisation methods for the approximate solution of the linear Fredholm integral equation of the first kind,

$$(1) \quad \int_a^b K(s, t) f(t) dt = g(s)$$

where $K(s, t)$ is a known (non-degenerate) symmetric $\mathcal{L}_2$ kernel. Here, the data function $g(s)$ is not known explicitly but is given by m discrete, and distinct, experimental observations $\{y(s_i)\}$ which may be contaminated by white-noise errors.

A general r -th order regularising functional describing an approximation $\hat{f}(t)$ to $f(t)$ in (1), may be written as

$$(2) \quad F_\lambda[\hat{f}] = \frac{1}{m} \sum_{i=1}^m \left(\mathcal{K} \hat{f}(s_i) - y(s_i) \right)^2 + \lambda \int_a^b \left[\hat{f}^{(r)}(t) \right]^2 dt$$

where $\mathcal{K}f(s) = \int_a^b K(s, t) f(t) dt$ and $r = 0, 1$ or 2 . If we define $\hat{f}(t)$ in the general linear form $\hat{f}(t) = \sum_{j=1}^n c_j \phi_j(t)$ then, assuming that the regularisation parameter λ is known, we may determine $\hat{f}(t)$ by minimisation of (2) with respect to the n coefficients $\{c_j\}$.

In this paper we describe an algorithm for computing the zero-order ($r = 0$) regularised solution $\hat{f}(t)$ using a basis of approximate eigenfunctions of the symmetric kernel $K(s, t)$, and the technique of Generalised Cross Validation for calculating an unbiased estimate to the optimum value of the parameter $\lambda > 0$. This novel algorithm has many advantages

over existing methods in general application, and these will be discussed. Numerical results obtained from application of the algorithm to model problems will also be presented.

STABILISED FINITE ELEMENT METHODS FOR STEADY INCOMPRESSIBLE FLOW

H Blank, M Rudgyard & A Wathen (*Oxford University, Computing Laboratory, Wolfson Building, Oxford OX1 3QD, UK*)

We study two families of stabilised finite element methods employed for steady incompressible flow: streamline upwind Petrov-Galerkin type methods (SUPG) and Taylor-Galerkin like schemes. These methods present an alternative to frequently applied finite element schemes which employ different order interpolation for the velocity and the pressure terms.

SUPG methods were first introduced by Hughes and Brooks, who studied the advection-diffusion equation as a model problem for the incompressible Navier-Stokes equations. SUPG-type methods are Galerkin schemes with additional correction terms to better capture the convective effects. Generalised SUPG-type schemes were developed for the incompressible Navier-Stokes equations and have also been applied to compressible flow. Taylor-Galerkin schemes were first introduced by Donea. They can be derived by introducing an iterated operator in a Lax-Wendroff style and by applying a Galerkin scheme to the modified equation.

It will be shown how SUPG-type methods can be interpreted as variants of Taylor-Galerkin schemes, and by doing so we hope to be able to develop an alternative framework in which SUPG methods may be understood. Even though Taylor-Galerkin methods are generally used for hyperbolic conservation laws, we will show how they can be applied to other types of partial differential equations. Both SUPG and Taylor-Galerkin schemes have in common that certain weighted stabilisation terms are added to traditional Galerkin schemes. However, we shall demonstrate that the terms employed by SUPG-type methods to stabilise effects of the incompressibility constraint of the Navier-Stokes equation correspond to second order terms of the Taylor-Galerkin scheme applied to the artificial compressibility equation.

We discuss natural boundary conditions, the choice of parameters, and we will present new numerical results.

REAL-TIME STATE ESTIMATION USING WAVELET TECHNIQUES

L Blank (*RWTH Aachen, Institut fuer Geometrie und Praktische Mathematik, Tempelgraben 55, 52056 Aachen, Germany*)

The real-time problem of state estimation is given as a optimization problem on a receding horizon with known noisy signals. The given noisy signals are treated with nonlinear algorithms based on wavelets. The optimization problem is reformulated as a variational problem. Discretization of this variational problem is then given by projection on finite dimensional wavelet-spaces. This ansatz gives a unified frame for signal analysis and optimization treatment. Furthermore, the wavelet concept enables at all steps of the applied iterative algorithm to update efficiently the approximative solution and the resulting system of discretized equations. This pursues the goal to have a best possible solution at any time during the a priori unknown available computation time, for which the dynamic of the plant only gives an upper bound. Finally, numerical examples are given. (The necessary background for wavelets is shortly introduced.)

FINITE ELEMENT APPROXIMATION OF A FOURTH ORDER NONLINEAR DEGENERATE PARABOLIC EQUATION

J F Blowey, J W Barratt & H Garcke (*University of Durham, Department of Mathematical Sciences, DH1 3LE, UK*)

We consider a fully practical finite element approximation of the fourth order nonlinear degenerate parabolic equation

$$u_t + \nabla \cdot (|u|^p \nabla \Delta u) = 0,$$

for any given $p \in (0, \infty)$. An iterative scheme for solving the resulting nonlinear algebraic system is analysed. In addition to showing well-posedness of our approximation, we prove convergence in one space dimension. Finally some numerical experiments are presented.

THE OPTIMAL WITH RESPECT TO ACCURACY, COMPLEXITY AND MEMORY ALGORITHMS OF CALCULATING SINGULAR INTEGRALS AND SOLUTIONS OF INTEGRAL EQUATIONS

I V Boikov (*Penza State Technical University, Department of Higher Mathematics, 40, Krasnaya Str, Penza, 440017, Russia*)

In the first part of the presentation we discuss the optimal by accuracy, complexity and memory algorithms of calculation of singular integrals of the following types

$$\begin{aligned} & \int_{-1}^1 \frac{x(t)}{t} dt, \quad \frac{1}{2\pi} \int_0^{2\pi} x(t) \operatorname{ctg} \frac{t-s}{2} dt, \quad \int_0^1 p(t) \frac{x(t)}{t-s} dt, \\ & \int_0^1 \int_0^1 \frac{x(\tau_1, \tau_2)}{(\tau_1 - t_1)(\tau_2 - t_2)} d\tau_1 d\tau_2, \quad \int_D \frac{f(q)x(u)}{r(u, v)} du, \end{aligned}$$

where $q = (u-v)/r(u, v)$, $u = (u_1, u_2)$, $v = (v_1, v_2)$, $r(u, v) = [(u_1 - v_1)^2 + (u_2 - v_2)^2]^{1/2}$, $D = [-1, 1; -1, 1]$

The optimal algorithms were constructed on the Holder and Sobolev classes of the functions. Some of these algorithms are asymptotically optimal by accuracy and optimal by order by complexity and memory and some of them are asymptotically optimal by complexity and optimal by order by accuracy and memory.

We also study the methods of calculation of the Hadamard finite-part integrals

$$\int_{-1}^1 \frac{f(t)dt}{(t-s)^p} \quad \int_{-1}^1 \int_{-1}^1 \frac{f(t_1, t_2)dt_1 dt_2}{(t_1 - s_1)^{p_1} (t_2 - s_2)^{p_2}} \quad \int_{-1}^1 \int_{-1}^1 \frac{f(t_1, t_2)dt_1 dt_2}{((t_1 - s_1)^2 + (t_2 - s_2)^2)^p}.$$

In the second part of the presentation we construct the approximate methods of decision of singular integral equations and integral equations with Hadamard integrals. We consider the one and many dimensional equations. We investigate the numerical methods of decision of the linear and nonlinear equations and equations which are determined on piecewise continuous contours.

We study the optimal by accuracy methods of decision of singular integral equations with Cauchy type kernels

$$a(s)x(s) + \int_l p(t) \frac{x(t)}{t-s} dt + \int_l h(s, t)x(t) dt = f(s),$$

polysingular integral equations and many dimensional singular integral equations. The estimates of accuracy and speed of convergence are received.

In the third part of the presentation we consider the applications of the singular integral equations to the inverse tasks of the geophysics and to some tasks of the aerodynamics.

CONVERGENCE ANALYSIS OF AN ITERATIVE APPROXIMATION METHOD FOR A NON-LINEAR VOLTERRA INTEGRAL EQUATION

E Buckwar (*Freie Universität Berlin, Department of Mathematics and Computer Science, Arnimallee 2-6, D - 14195 Berlin, Germany*)

In this talk an approximation method for a nonlinear Volterra integral equation of convolution type is considered. The equation has at least the trivial solution, but one is interested in a continuous, positive solution. In order to obtain a numerical approximation of the non-trivial solution the method of successive approximations has been discretized, where the integral is replaced by numerical quadrature. The speaker will present the convergence analysis for this method, based on a fixed point theorem in cones in Banach spaces and the concept of discrete approximations. In contrast to the usual approach nonlinear restriction and prolongation operators are used. Results of numerical experiments are demonstrated.

IDENTIFYING LINEAR COMBINATIONS OF RIDGE FUNCTIONS

M Buhmann & A Pinkus (*University of Dortmund, FB Mathematik, Lehrstuhl 8 44221 Dortmund, Germany*)

A *ridge function*, in its simplest shape, is a multivariate function

$$h : \mathcal{R}^n \rightarrow \mathcal{R}$$

of the form

$$h(x_1, \dots, x_n) = g(a_1x_1 + \dots + a_nx_n) = g(a \cdot x)$$

where $g : \mathcal{R} \rightarrow \mathcal{R}$ and $a = (a_1, \dots, a_n) \in \mathcal{R}^n \setminus \{0\}$. In other words, it is a multivariate function constant on the parallel hyperplanes $a \cdot x = c$, $c \in \mathcal{R}$. The vector $a \in \mathcal{R}^n \setminus \{0\}$ is generally called the *direction*.

Ridge functions appear in various areas and under various guises. We find them in the area of partial differential equations (where they have been known under the name of plane waves), in statistics (where they appear in projection pursuit algorithms) and in neural networks.

In this talk, we assume we are given a function $f(x)$ which we know to be a sum of ridge functions $\sum_{i=1}^m g_i(a^i \cdot x)$. We seek to identify—from knowing only f —the functions g_i and also the directions a^i . We will show how this nonlinear problem can be solved in certain cases.

MODELLING AND SOLUTION OF OPTIMIZATION PROBLEMS WITH DIFFERENTIAL EQUATION CONSTRAINTS

G Burnside & R Middleton (*University of Dundee, Department of Mathematics & CS, Dundee, DD1 4HN, UK*)

The solution of nonlinear optimization problems with differential algebraic equation (DAE) constraints is considered. These arise in many fields, including chemical engineering and trajectory problems. A new modelling language for the description of this

type of problem is being developed. This language is based on OTL, which is designed for the modelling of nonlinear programming problems. Existing modelling packages such as CUTE and AMPL do not allow the modelling of DAE constraints. The problems are solved by approximating the functions using collocation over finite elements resulting in large nonlinear programming problems. These discretized problems are solved by a sequential quadratic programming method. The discretization is then refined using an iterative scheme.

ERROR GROWTH WHEN SYMMETRIC MULTISTEP METHODS INTEGRATE PERIODIC ORBITS OF REVERSIBLE SYSTEMS

B Cano (*Universidad de Valladolid, Departamento de Matematica Aplicada y Computacion, 47005-Valladolid, Spain*)

We show why symmetric linear multistep methods are not suitable for the integration of reversible first order problems in spite of the good properties shown by their one-step counterparts [1]. However, symmetric multistep methods specially designed for second order problems and without parasitic double roots turn out to be very useful.

[1] Cano, B. & Sanz-Serna, J. M., 1995, "Error growth in the numerical integration of periodic orbits, with application to Hamiltonian and reversible systems" *SIAM J. Num. Anal.* to appear.

NEW METHODS OF SYMPLECTIC INTEGRATION WITH PROCESSING

F Casas, S Blanes & J Ros (*Universitat Jaume I, Departament de Matemàtiques, 12071-Castellón, Spain*)

In this communication we carry out a general analysis of the explicit symplectic integrators with processing for a Hamiltonian of the form $H = A + B$, where $\exp(-hA)$, $\exp(-hB)$ can both be calculated explicitly. More specifically, we analyse numerical integrators defined by $\exp(P)\exp(-hK)\exp(-P)$, in which the kernel $\exp(-hK)$ and the processor $\exp(P)$ are both compositions of the elementary flows $\exp(-haA)$ and $\exp(-hbB)$. In particular, we derive the conditions to be satisfied by the operator K and the equations to be solved for the processor up to order 6. As a result, we obtain new symplectic integration algorithms of order 4, 5, and 6 with 3, 4, and 5 evaluations of $\exp(-hB)$, respectively, which are more efficient than previous symplectic methods.

DISCRETE QMR AND BCG IN THE NUMERICAL SOLUTION OF LINEAR SYSTEMS OF ODEs

E Celledoni (*University of Cambridge, DAMTP, UK*)

We consider the use of QMR and BCG in the numerical solution of linear systems of ODEs reformulated as second kind integral equations. The implementation of the methods is performed in practice applying them on suitably discretized equations. An important issue in this context is to compare the behaviour of the discrete and continue iteration. Here we consider the case of linear systems of ODEs. The discretization is performed using a continuous Runge-Kutta method.

MODIFYING THE INERTIA OF MATRICES ARISING IN OPTIMIZATION

S H Cheng & N J Higham (*University of Manchester, Department of Mathematics, Manchester M13 9PL, UK*)

Applications in constrained optimization produce symmetric matrices with a natural block 2-by-2 structure. An optimality condition leads to the problem of perturbing the (1,1) block of the matrix to achieve a specific inertia. We derive a perturbation of minimal norm, valid for any unitarily invariant norm, that increases the number of nonnegative eigenvalues by a given amount, and we show how it can be computed efficiently given a factorization of the original matrix. We also consider an alternative way to satisfy the optimality condition based on a null space projection approach.

EXPLICIT SCHEMES FOR NONLINEAR SCHRÖDINGER EQUATIONS

R Ciegis (*Institute of Mathematics and Informatics, Akademijos 4, 2600 Vilnius, Lithuania*)

In this paper we consider the symmetrical three step Euler scheme and the DuFort–Frankel-type method for nonlinear Schrödinger equation

$$\frac{\partial U}{\partial t} = i \sum_{k=1}^d \frac{\partial}{\partial x_k} (a_k(x) \frac{\partial u}{\partial x_k}) + f(u, x, t).$$

The discrete conservation laws for both difference schemes are investigated. Convergence in the L_2 and L_∞ norms is proved for $d \geq 3$.

The stability of difference schemes is investigated by energy and spectral methods. Numerical results for cubic nonlinear Schrödinger equation are given. A comparison with the Crank–Nicolson method is given.

A NUMERICAL STUDY OF A NONLINEAR CHEMICAL OSCILLATOR VIA FINITE DIFFERENCES

A Cinar & E H Twizell (*Brunel University, Department of Mathematics and Statistics, Uxbridge UB8 3PH, UK*)

A mathematical model of a two-cell coupled non-linear isothermal chemical reactor problem is solved using finite-difference methods. In analysing the qualitative character of the reaction kinetics, multiple stationary states are observed with a Hopf bifurcation occurring and leading to complex dynamical behaviours.

First- and second-order numerical methods are proposed for the solution of this non-linear ODE system. The second-order numerical methods are developed by taking a linear combination of the appropriate first-order methods. These explicit finite-difference methods are compared in terms of linear stability. It is seen that especially the second-order numerical methods, show good stability properties and numerical simulations reflect the behaviour of the continuous-time system accurately.

INVARIANT ADAPTIVE DOMAIN SCHEMES FOR PARABOLIC PDES

G Collins & C J Budd (*University of Bristol, School of Mathematics, Bristol BS8 1TW, UK*)

Many PDE problems have Lie groups of transformations that leave them as well as certain quantities invariant. These quantities can be regarded as the natural scalings of the PDE problem and are used as similarity variables in the construction of similarity solutions. Invariants can also be used as computational variables in the construction of a moving mesh scheme based upon equidistribution. In fact it is shown that there is an important

commuting relation between a discretised scale-reduced PDE and a rescaled discretised PDE. This relation only holds if the PDE is solved on a moving mesh and the equation governing the movement of the mesh for the scheme is invariant to the given group.

This talk will show how Cauchy problems for PDE's that have such Lie groups are solved on an infinite domain by adapting the computational domain.

For example the Nonlinear diffusion equation, $u_t = (u^m u_x)_x$, has a group of stretching transformations that leave the PDE and a conservation law invariant. Two invariants of the group are, $xt^{-1/(m+2)}$ and $ut^{1/(m+2)}$. These invariants are also used to reduce the PDE to its principal ODE which is integrated twice to give the well known similarity solutions for the nonlinear diffusion equation.

To solve the PDE problem numerically using the method of lines, conditions are placed on the first and last nodes of the scheme so that the mesh will stretch in an appropriate way to follow the solution as it diffuses. The equations governing the mesh movement are invariant to the same group of transformations that the PDE is. It is shown that the invariants of the PDE are reproduced in the discretised scheme so that the mesh $X_i(t) = Y_i t^{1/(m+2)}$ and the computed solution $U_i(t) = V(Y_i) t^{1/(m+2)} = V_i t^{1/(m+2)}$ where Y_i and V_i are constants with respect to t .

In the analysis of the scheme it is easily seen that this 'natural' choice of mesh equation gives some nice properties concerning the dynamics of the discretised scheme in that there is a reduction of the system which is a discrete analogy to the similarity reduction. Stability and convergence proofs, which are generally lacking for moving mesh schemes, are more manageable for the reduced scheme. It is shown that the scheme compares favourably with alternative mesh schemes and fixed mesh methods.

Finally the scheme is extended to harder problems where conservation laws are used to follow travelling waves and to blow up problems where adapting the computational domain gives a truly invariant mesh.

ACCURACY AND STABILITY OF THE NULL SPACE METHOD FOR SOLVING THE EQUALITY CONSTRAINED LEAST SQUARES PROBLEM

A J Cox & N J Higham (*University of Manchester, Department of Mathematics, Manchester M13 9PL, UK*)

In this talk, we consider the least squares solution of an overdetermined system $Ax = b$ of linear equations subject to a system $Bx = d$ of linear equality constraints. First, we analyse the numerical stability of three variations of the null space method. Then we present improved perturbation bounds for the problem, and show how the generalized QR factorization may be used to compute them efficiently. We discuss the backward error of an arbitrary approximate solution of an equality constrained least squares problem. Finally, we present numerical results.

NUMERICAL INVERSION OF LAPLACE TRANSFORMS: A SURVEY AND COMPARISON OF THREE METHODS FOR THE REAL INVERSION PROBLEM

L D'Amore, Almerico Murli & M Rizzardi (*Center for Research on Parallel Computing and Supercomputers, CPS-CNR, Naples, Complesso Monte S. Angelo, Via Cintia, 80126 Napoli, Italy*)

We describe recent developments related to the numerical inversion of a Laplace Trans-

form function:

$$F(s) = \int_0^{\infty} e^{-st} f(t) dt, \quad \operatorname{Re}(s) > \sigma_0$$

when the data function is known on the real axis only; the inverse problem is the reconstruction of the original function $f(t)$ from known values of $F(s)$. Such problem is much more “difficult” to be solved due to an intrinsic ill-posedness of the (real) problem. The ill-posedness of the continuous problem is reflected into the ill-conditioning of the discrete problem.

The classical way to compute a stable solution is to *regularize* the problem. Today the theoretical basis for the solution of ill-posed problems, based on Tikhonov regularization, are very well stated. In spite of this progress on theoretical side, computational aspects have not found a comparable attention. This lack of algorithmic development is especially disappointing as more and more real-world problems need to be considered, or require real-time solutions, so that the very straightforward, simple implementation of the basic algorithms no longer fulfills the computational requirements. Nowadays the term *regularization* characterizes any computational strategy that leads to “useful” solution by introducing some kind of filtering and provides robust methods for choosing the optimal weight given to the regularization process.

The underlying idea of the present work is to point out these computational features in the numerical inversion of the Laplace transform, in order to put them together in one common framework, and to provide useful guidelines in the development of efficient and stable algorithms. Our attention has been devoted to the analysis of three discretization schemes which we consider the most promising ones, in terms of accuracy and efficiency and, by introducing some kind of filtering, we show their effectiveness when applied in the real inversion framework.

ON THE STATIONARY AND NON-STATIONARY EXTRAPOLATION ITERATIVE METHOD

D S Daoud (*Eastern Mediterranean University, Department of Mathematics, G-Magusa, via: Mersin 10, North Cyprus*)

In this article theoretical results are presented on the extrapolation of the first order iterative method to estimate the optimal value of the extrapolation parameter together with the rate of convergence which depends inversely on the p -condition number of the coefficient matrix.

A further extension is considered to define a non-stationary extrapolation method with a changeable extrapolation parameter at each iteration step.

For the non-stationary type it has a faster rate of convergence than the stationary type which depends inversely on $p^{1/2}$, the extrapolation parameters are also estimated using Tchebysev polynomials.

The stationary and non-stationary extrapolation methods are considered for the Jacobi and SOR methods.

MODELLING AND NUMERICS FOR KEYHOLE SURGERY SIMULATIONS

P J Davies, F J Carter & A Cuschieri (*University of Strathclyde, Department of Mathematics, Glasgow G1 1XH, UK*)

Surgeons receive special training in order to practice endoscopic or “keyhole” surgery. Much of their training is carried out on hollow dummies, supplemented by videos of real

operations. This approach can be expensive and has limitations. I am part of a group working on a project whose long-term aim is to produce a computer training package that simulates abdominal keyhole surgery.

The main mathematical obstacles to be overcome in order to create such a package are to find realistic (nonlinearly elastic) biomechanical models for intestinal tissue, and then to design numerical methods suitable for solving the complicated boundary value problems corresponding to interactions between the tissue and surgical instruments. I shall describe some of the experimental and numerical techniques that we are using to do this.

LAGRANGE AND HERMITE INTERPOLATION POINTS FOR C^1 QUARTIC BIVARIATE SPLINES

O Davydov (*Dnepropetrovsk State University, Department of Mechanics and Mathematics, Gagarina 72, Dnepropetrovsk, GSP 320625, Ukraine*)

Let $\Omega \subset \mathbb{R}^2$ be a connected polygonal domain, and let $\Delta = \{T_1, \dots, T_N\}$ denote a triangulation of Ω . The space of quartic bivariate polynomial splines of smoothness 1 with respect to Δ is defined by

$$S_4^1(\Delta) := \{s \in C^1(\Omega) : s|_{T_i} \in \Pi_4, i = 1, \dots, N\},$$

where

$$\Pi_4 := \text{span} \{x^i y^j \text{ st. } i \geq 0, j \geq 0, i + j \leq 4\}$$

is the space of bivariate polynomials of total degree 4.

The space $S_4^1(\Delta)$ was studied in [1], where the dimension and an explicit basis for it were found. However, it was an open question whether the functions in $S_4^1(\Delta)$ could be used to interpolate to given function and gradient values at all vertices of the triangulation Δ (see [1, Remark 3]).

We give an affirmative answer to this question. Moreover, we obtain Lagrange and Hermite interpolation schemes for $S_4^1(\Delta)$, give a new proof of the dimension result of [1] and construct basis functions for $S_4^1(\Delta)$ with relatively small supports.

[1] P. Alfeld, B. Piper and L. L. Schumaker, An explicit basis for C^1 quartic bivariate splines, *SIAM J. Numer. Anal.* **24** (1987), 891–911.

SOLUTION OF STRUCTURED SYSTEMS OF LINEAR EQUATIONS USING SUBSPACE-BY-SUBSPACE PRECONDITIONERS

J P Décamps, M J Daydé & N I M Gould (*ENSEEIH-IRIT, Toulouse, 2 rue Camichel, 31071 Toulouse CEDEX, France*)

We consider the iterative solution of symmetric positive-definite linear systems whose coefficient matrix may be expressed as the sum of outer-products of low-rank terms. We derive suitable Subspace-by-Subspace preconditioners for such systems, and demonstrate their effectiveness on a number of test examples arising from least-square problems.

We also show how to combine Subspace-by-Subspace preconditioners with classical Element-by-Element preconditioners to obtain effective preconditioners for "partially separable" linear systems where the elementary matrices are not all of low-rank.

NUMERICAL TREATMENT OF FRACTIONAL DIFFERENTIAL EQUATIONS

K Diethelm (*Universität Hildesheim, Institut für Mathematik, Marienburger Platz 22, 31141 Hildesheim, Germany*)

We consider the differential equation

$$(1) \quad D^q y = \alpha y + f$$

where $0 < q < 1$ with the initial condition $y(0) = 0$ on the interval $[0, 1]$. Here, D^q is the q th order differential operator in the sense of Riemann and Liouville. Whereas the applications of (1) to diffusion processes are known for quite some time now, it has been shown in recent years that (1) may also be used for the modelling of damping laws, the relaxation of proteins and polymers, and many other processes.

We shall solve the differential equation with a method corresponding to the trapezoidal method. It turns out that classical techniques can be used to prove the stability of the method. However, on the questions of convergence, only rather weak results can be obtained in this way. Using new sharp error bounds for a related quadrature problem, we can improve these results and derive a uniform error bound of the order h^{2-q} .

We will also discuss various possible generalizations and modifications of this approach that may be used to construct methods with improved convergence properties.

SOLUTION OF SPARSE QUASI-SQUARE SYSTEMS IN MULTIBODY KINEMATICS

I S Duff, J Cardenal & J M Jimenez (*Rutherford Appleton Laboratory and CERFACS, Didcot, OX11 0QX, UK*)

We discuss the solution of least-squares and minimum-norm solutions of rectangular systems that arise in multibody kinematic problems. A characteristic of the matrices from this application is that they are rectangular but have almost the same number of rows and columns. We call such systems quasi-square and discuss a direct method based on LU factorization of the rectangular matrix that is particularly efficient on such systems. We find that this approach is far superior to using normal equations or Peters and Wilkinson's method and that good advantage can be taken of sparsity. We also show that the structure of these problems leads to an amusing result in the factorization of the augmented system. We illustrate our talk by the solution of some practical problems in multibody kinematics.

APPROXIMATING A NONLINEAR INTEGRO-PARTIAL DIFFERENTIAL EQUATION

D B Duncan & A R Soheili (*Heriot-Watt University, Department of Mathematics, Edinburgh EH14 4AS, UK*)

Coagulation processes such as the formation of aerosols, gels and galaxies are often modelled by the Smoluchowski equation

$$\frac{\partial u(\nu, t)}{\partial t} = \frac{1}{2} \int_0^\nu \beta(\mu, \nu - \mu) u(\mu) u(\nu - \mu) d\mu - u(\nu) \int_0^\infty \beta(\mu, \nu) u(\mu) d\mu$$

where t is time, $\nu > 0$ is the particle size and $u(\nu, t)$ is the number of particles of size ν . The function $\beta(\mu, \nu)$ is the collision frequency factor between particles of size μ and ν , and contains much of the information about the physics of the process.

In this talk we describe how to construct an approximation of this integro-PDE in some particular cases, using a fast method for the integrals and a PDE-type moving mesh technique to follow the solution as the average particle size increases.

ERROR GROWTH IN CONSERVATIVE NUMERICAL METHODS FOR THE NONLINEAR SCHRÖDINGER EQUATION

A Durán (*Universidad de Valladolid, Departamento de Matematica Aplicada y Computacion, Spain*)

One of the relevant properties of numerical methods for integrating time-dependent differential equations is the conservation of physical quantities that remain constant during the evolution of the system. Some recent results [1] show the influence of the conservative nature of the algorithms on the accuracy of the numerical solution.

We consider solitary wave problems for the Nonlinear Schroedinger equation and show that, at leading order, the use of conservative numerical schemes makes the error increase with time in a different way from that for nonconservative methods. Numerical experiments are presented.

[1] J. de Frutos, J.M. Sanz-Serna, "Accuracy and Conservation Properties in Numerical Integration: the Case of the Korteweg-de Vries Equation" *Numer. Math.* 75: 421-445 (1997).

INTEGRATING COMPOSED SINGULARITIES USING NON-UNIFORM SUBDIVISION AND EXTRAPOLATION

T O Espelid & K Singstad (*University of Bergen, Department of Informatics, Høyteknologisteret, N-5020 Bergen, Norway*)

An approach to the computation of approximations to multidimensional integrals over an n -dimensional hyper-rectangular region, when the integrand has a composed singularity, is described. This approach is based on a non-uniform subdivision of the region of integration and the technique fits well to the sub-division strategy used in many adaptive algorithms. The technique turns out to have good numerical stability properties. A two dimensional experimental code is used to demonstrate the power of this approach.

A GENERALIZED METHOD FOR IRREGULAR OSCILLATORY QUADRATURE

G A Evans (*De Montford University, Department of Mathematics, James Went Building, Leicester LE1 9BH, UK*)

The irregular oscillatory integral

$$\int_a^b f(x) g(q(x)) dx$$

where $g(\xi)$ is an oscillatory function such as $\sin(\xi)$ or $J_n(\xi)$, and the argument $q(x)$ represents the irregular part, can now be integrated numerically using a stable high order method. By considering $g(q(x))$ as being the solution of a linear second order differential equation, a generalised approach can be derived which naturally encompasses the trigonometric method of Evans and Webster[1996] and allows obvious extensions to Bessel function oscillations, and to combinations of Bessel and trigonometric weights. It also appears that infinite range oscillatory integrals can be encompassed in this work and investigations continue to find further useful cases and relate the approach to the classic method of variation of the parameters. The possibility of using higher order differential equations then arises.

UPPER-SEMICONTINUITY OF ATTRACTORS FOR A PSEUDOSPECTRAL APPROXIMATION OF THE KURAMOTO-SIVASHINSKY EQUATION

M A Falcon (*University of Bath, School of Mathematics, Bath BA2 7AY, UK*)

We formulate semi-discrete approximations to the Kuramoto-Sivashinsky equation using a pseudospectral method. We prove that these approximations are in a discrete Gevrey class, which allows us to prove the existence of attractors for these approximations. Upper-semicontinuity of these approximate attractors to the continuous global attractor of the Kuramoto-Sivashinsky is then established as the approximation is refined.

VOLTERRA INTEGRAL EQUATIONS WITH NON-LIPSCHITZ NONLINEARITY

N J Ford, J T Edwards & K Frischmuth (*University College Chester, Department of Mathematics, Chester CH1 4BJ, UK*)

In this work we consider equations of the form:

$$y(t) = g(t) + \int_0^t k(t-s)\varphi(y(s))ds, \quad t \in \mathbb{R}^+,$$

when solved analytically and numerically. Some recent work has considered the qualitative behaviour of solutions of equations of this form. In the present work, we consider examples which do not satisfy classical conditions guaranteeing existence and uniqueness of the exact solutions and suitable behaviour of approximate solutions. We are able to give a strengthened version of a theorem given originally by Corduneanu for certain kernels and nonlinearities. On that basis we consider how certain numerical codes may fail. We explore and test methods known to preserve properties of the solutions in the linear case.

THE PSEUDOSPECTRAL ELEMENT METHOD FOR ONE-DIMENSIONAL HYPERBOLIC SYSTEMS

B Fornberg & T Driscoll (*University of Colorado, Boulder, Dept. of Applied Mathematics, CO 80309-0526, USA*)

In the pseudospectral element (PSE) method, the coupling between subdomains is achieved by derivative matching along boundaries. Compared to spectral elements coupled through characteristics, the PSE method offers both better stability and accuracy, especially in cases of discontinuous coefficients. Computational examples for Maxwell's equations show that PSE retains high accuracy over times orders of magnitude longer than not only low-order methods (such as Yee's), but also over high-order methods, such as characteristics-based spectral elements.

PROPERTIES OF GAUSSIAN ELIMINATION WITH ROOK PIVOTING

L Foster (*San Jose State University, Department of Mathematics & Computer Science, San Jose, CA 95192, USA*)

Gaussian elimination is among the most widely used tools in scientific computing. Gaussian elimination with partial pivoting requires only $O(n^2)$ comparisons beyond the work required in Gaussian elimination with no pivoting but can, in principle, have error growth that is exponential in the matrix size n . Gaussian elimination with complete pivoting, on the other hand, can not have exponential error growth but requires $O(n^3)$ comparisons beyond the work required by Gaussian elimination with no pivoting. Gaussian elimination with rook pivoting is a technique that appears to be intermediate between partial pivoting and complete pivoting in term of efficiency and accuracy. We prove that rook pivoting can not have exponential error growth and we show that in practice rook

pivoting usually requires $O(n^2)$ comparisons beyond the work required by Gaussian elimination with no pivoting. We also discuss a combination of partial pivoting and rook pivoting that implements rook pivoting only when the growth factor for partial pivoting is large. This combination can not have exponential error growth and appears to require the same computer time as a partial pivoting algorithm that calculates the growth factor. Finally we show that rook pivoting produces rank revealing factorizations when partial pivoting fails to do so.

ON SPECTRAL VALUE SETS FOR INFINITE DIMENSIONAL SYSTEMS

E Gallestey, D Hinrichsen & A J Pritchard (*Universität Bremen, Institut für Dynamische Systeme, D-28334 Bremen, Germany*)

We study how the spectrum of closed linear operators on infinite dimensional spaces change under the effect of perturbations. The spectral value set that can be achieved by perturbations of a given level is characterized in terms of the norm of a transfer function $\|G(\lambda)\|$, $\lambda \in C$. In order to compute the sets finite dimensional approximations must be made. We define the approximation problem and illustrate some of the difficulties by applications to a delay equation and the Orr-Sommerfeld equation.

AIM POSTPROCESSING FOR DISSIPATIVE PDES: THE FINITE-ELEMENT CASE

B García-Archilla & E S Titi (*Universidad Autónoma de Madrid, Departamento de Matemáticas, 28049 Madrid, Spain*)

Recently, a technique to improve the accuracy of classical Galerkin (and related) methods has been introduced [2], [3], [4]. This technique raises the approximate Galerkin solution to the Foias-Manley-Temam approximate inertial manifold (AIM) [1], and so far, has been applied with spectral and pseudospectral methods. In the present paper we present the extension of AIM postprocessing to Finite-Element methods. The postprocessed methods possess higher orders of convergence than the classical methods on which they are based, and this enhancement is achieved at practically no computational cost. We present numerical experiments that suggest that the AIM-postprocessed Finite-Element methods are computationally more efficient not only than the classical methods on which they are based, but also than methods with the same convergence rate.

[1] C. Foias, O. Manley and R. Temam, Modelling of the interaction of small and large eddies in two dimensional turbulent flows, *RAIRO M²AN*, **22** (1988), pp. 93–114.

[2] J. de Frutos, B. García-Archilla and J. Novo, A postprocessed Galerkin method with Chebyshev and Legendre polynomials, (submitted).

[3] B. García-Archilla, J. Novo and E. S. Titi, Postprocessing the Galerkin method: a novel approach to approximate inertial manifolds, *SIAM J. Numer. Anal.* (to appear).

[4] B. García-Archilla, J. Novo and E. S. Titi, An approximate inertial manifold approach to postprocessing Galerkin methods for the Navier-Stokes equations, (submitted).

A MIXED SPECTRAL ELEMENT METHOD FOR CREEPING FLOWS USING A DOUBLY CONSTRAINED MINIMIZATION APPROACH

M I Gerritsma & T N Phillips (*University College of Wales, Aberystwyth, Dept of Applied Mathematics, Penglais, Aberystwyth, SY23 3BZ, UK*)

The approach adopted in this work is to minimize the viscous stress tensor τ in a weak sense subject to the constraint that the viscous forces are irrotational. This constrained

minimization problem leads to the introduction of the Lagrange multiplier $\mathbf{w}$, in physical terms the fluid velocity, which itself is constrained by the condition that $\nabla \cdot \mathbf{w} = 0$, which describes the incompressibility of the fluid, and appropriately chosen boundary conditions. This leads to a second Lagrange multiplier p , known as the pressure. So here one has a constraint in a constraint.

Usually the stress tensor is eliminated from this set of equations and the whole problem is stated in terms of $\mathbf{w}$ and p . However, for more complex constitutive equations this is not always possible, so it is very instructive to consider the mixed formulation given above.

It is possible to analyze the two constraints and its Lagrange multipliers separately. In the discrete case the first constraint requires that the velocity field and the the field of the stress tensor are compatible, whereas the second constraint requires a pressure field which should be compatible with the velocity field. Although much attention has been given to the velocity-pressure relation in finite element and spectral element theory not much is known about the the stress-velocity relation.

The hierarchy of nested constraints will be presented and in the case of the spectral element method the relation between the different function spaces will be given, based on the Babuška-Brezzi criteria for mixed methods.

A comparison between the mixed approach and the standard primitive variable formulation will be made in terms of the condition number of the resulting systems in several flow geometries. The application of the mixed formulation to a nonlinear constitutive relationship, the upper-convected Maxwell model, is discussed.

CLOSED LOOP DESIGN FOR A SIMPLE NONLINEAR AIRCRAFT MODEL USING EIGEN-STRUCTURE ASSIGNMENT

L P Gibson & N K Nichols (*University of Reading, Department of Mathematics, UK*)

Aircraft systems are highly nonlinear and time varying. High performance aircraft at high angles of incidence experience undesired coupling of the lateral and longitudinal variables, resulting in departure from normal controlled flight. The aim of this work is to construct a robust closed loop control that optimally extends the stable and decoupled flight over the control parameter space. For the study of these systems nonlinear analysis methods are needed. Previously, bifurcation techniques have been used mainly to analyse open loop nonlinear aircraft models and investigate control effects on dynamic behaviour. In this work linear feedback control designs calculated by eigenstructure assignment methods are investigated for a simple aircraft model at a fixed flight condition. Bifurcation analysis in conjunction with linear control design methods is shown to aid control law design for the nonlinear system.

WATER WAVE PROBLEMS: WHAT WE REALLY REALLY WANT

J Goodwin (*University of Reading, Department of Mathematics, Reading, UK*)

Building a physical model is an expensive way of predicting water wave behaviour over undulating topography and around breakwaters; a numerical model is the attractive alternative. However, there are difficulties faced by numerical approaches. Just as with the physical model, the problem domain is essentially infinite and needs to be limited to an appropriate finite region, without introducing spurious effects by its boundaries. The numerical problem can also demand a dense grid to ensure accurate wave represen-

tation. A numerical method is presented which is based on recent developments in water wave approximation; global boundary conditions are implemented to limit domain size effectively and the 'mild-slope' class of water wave approximations is used to reduce the problem from three dimensions to two, whilst efficiently modelling both refraction and diffraction phenomena. The method is applied to several test problems, demonstrating that it is an important first step towards a practical numerical solver.

SOLVING THE TRUST-REGION SUBPROBLEM USING THE LANCZOS METHOD

N I M Gould (*Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK*)

The approximate minimization of a quadratic function within an ellipsoidal trust region is an important subproblem for many nonlinear programming methods. When the number of variables is large, the most widely-used strategy is to trace the path of conjugate gradient iterates either to convergence or until it reaches the trust-region boundary. In this paper, we investigate ways of continuing the process once the boundary has been encountered. The key is to observe that the trust-region problem within the currently generated Krylov subspace has very special structure which enables it to be solved very efficiently. We compare the new strategy with existing methods. The resulting software package is available as HSL_VF05 within the Harwell Subroutine Library.

HYBRID GALERKIN BOUNDARY ELEMENT METHODS

I G Graham, W Hackbusch & S Sauter (*University of Bath, School of Mathematical Sciences, Bath BA2 7AY, UK*)

Boundary element methods are popular for the solution of many PDEs, especially those describing classical problems in mechanics in complicated 3D regions. Their implementation poses two problems not found in the finite element method. Firstly the assembly of the stiffness matrices requires computation of singular integrals on surfaces and secondly the resulting matrices are full and may not have structure convenient for the implementation of standard iterative methods. There is much recent work on the second difficulty (multipole, panel-clustering, wavelet bases, preconditioning, etc). However the first difficulty remains: for moderate-sized discretisations the matrix assembly process can often form the dominant part of the computation.

In this work we describe a new quadrature method for computing stiffness matrices arising from piecewise linear Galerkin discretisations of a wide class of integral operators. For most of the matrix entries the method uses kernel evaluations at node points of the mesh only (rather than interior points of elements) and because of this it reduces the complexity of the computation of matrix entries away from the diagonal by a factor of about $1/64$.

Viewed in a different way the new method computes sufficiently accurate approximations of the Galerkin matrix away from the main diagonal using only appropriately averaged values of a certain (cheap) discrete collocation matrix. Hence the term "hybrid Galerkin method".

We are able to prove that the resulting numerical solution enjoys the same asymptotic convergence properties in the energy norm as the Galerkin method itself. The proof allows locally refined non-quasiuniform meshes such as those which may be used in the approximation of solutions with singularities.

ITERATIVE-COLLOCATION METHOD OF SOLVING VOLTERRA-FREDHOLM INTEGRAL EQUATIONS

L Hącia (*Technical University of Poznan, Institute of Mathematics, Piotrowo 3a, 60-965 Poznan, Poland*)

The Volterra-Fredholm integral equation

$$u(x, t) = f(x, t) + \int_0^t \int_M k(x, t; y, s) u(y, s) dy ds$$

is solved by the following iterative-collocation method

$$u_n(x, t) = f(x, t) + \int_0^t \int_M k(x, t; y, s) [u_{n-1}(y, s) + w_n(y, s)] dy ds, \quad n = 1, 2, 3, \dots,$$

where the corrections $w_n(x, t)$ are interpolation polynomials of the Lagrange type respect to variable $x \in M$, for every $t \in [0, T]$, of the form

$$\omega_n(x, t) = \sum_{j=0}^N a_j^{(n)}(t) \varphi_j(x),$$

with

$$\begin{aligned} \omega_n(x_i, t) &= u_n(x_i, t) - u_{n-1}(x_i, t), \quad i = 0, 1, 2, \dots, N, \\ \varphi_j(x_i) &= \delta_{ij}. \end{aligned}$$

The functions $a_j^{(n)}(t)$ are unique solution of a certain system of Volterra integral equations. The convergence of this algorithm is proved and an error estimate is established. The given theory is illustrated by numerical examples.

STABLE DIFFERENTIATION FORMULAS

M Hegland & R S Anderssen (*Australian National University, Computer Sci. Lab., RSISE, CANBERRA ACT 0200, Australia*)

While finite difference approximations have been very successfully applied for the solution of differential equations they can give disastrous results if used for computing derivatives from measured data. The reason for this is that measurement errors are strongly amplified in particular if small step sizes are used and higher order derivatives are computed. Based on earlier work by Anderssen and de Hoog new finite difference approximations have been developed which combine averaging with sampling to obtain stable and convergent differentiation formulas.

For example, a stable formula for the first derivative of $f(x)$, which can be applied to measurements y_i of $f(x_i)$ with $x_i = ih, i = 1, \dots, n$, uses the average

$$\bar{y}_i = \frac{y_{i-r} + \dots + y_{i+r}}{2r + 1}$$

in conjunction with the mid-point rule to yield an approximation $\dot{\bar{y}}_i$ of the derivative $f'(x_i)$ as

$$\dot{\bar{y}}_i = \frac{\bar{y}_{i+k} - \bar{y}_{i-k}}{2kh}.$$

The parameters k and r are chosen in order to guarantee that the resulting formula is stable. This stability is achieved by forcing the approximation error to be slightly less than $O(h^2)$. The nature of this trade-off as well as the choice of the parameters k and r will be discussed. Furthermore, the application of these results to higher order and partial derivatives will be examined and several applications of numerical differentiation will be presented. Some of the work was done jointly with Frank de Hoog, CSIRO.

HYPERBOLIC PROBLEMS WITH SOURCE TERMS, PART I: RUNGE–KUTTA TIMESTEP- PING

D J Higham, M A Aves & D F Griffiths (*University of Strathclyde, Department of Mathematics, Glasgow G1 1XH, UK*)

It is well known that Runge–Kutta methods applied to nonlinear ordinary differential equations may admit spurious fixed points. Here, we consider a linear advection equation with nonlinear source term. We use upwinding in space and we time-step with a two-stage explicit Runge–Kutta method. We show how the concept of a spurious fixed point extends to this setting and we give examples of undesirable long-term solutions. We also discuss the extent to which adaption in either space or time eliminates spurious behaviour.

ELLIPTIC AND PARABOLIC ESTIMATES

A T Hill (*University of Bath, School of Mathematical Sciences, UK*)

Consider the elliptic boundary value problem

$$(L + c)[u] = f, \quad x \in \Omega, \quad u(\partial\Omega) = 0,$$

for bounded $\Omega \subset \mathbb{R}^N$, where L is of the form

$$L[u] = -a_{ij}(x)D_iD_ju + b_i(x)D_iu, \quad \text{or } L[u] = -D_i(a_{ij}(x)D_ju) + b_iD_iu,$$

or the adjoint of one of these operators, with advection in conservation form.

Suppose that U is a numerical solution of such a problem, defined in all of Ω (and not just at nodes). Then $e = u - U$ satisfies the residual equation

$$(L + c)[e] = r \equiv f - (L + c)[U],$$

where the right-hand side is, in principle, computable. As a result, one obtains the *a posteriori* error estimate

$$\|e\|_X \leq \|(L + c)^{-1}\|_{\mathcal{L}(Y, X)} \|r\|_Y.$$

In this talk we present work estimating $\|(L + c)^{-1}\|_{\mathcal{L}(Y, X)}$, which is often not available from computations. Under the assumptions that

$$a_{ij}(x)\xi_i\xi_j \geq |\xi|^2; \quad \sqrt{\sum_{i=1}^N b_i^2(x)} \leq M; \quad c(x) \geq \lambda \geq 0,$$

we obtain rigorous explicit sharp upper bounds in the case $X = L_p(\Omega)$, $Y = L_q(\Omega)$, $1 \leq p, q \leq \infty$. When $\lambda = 0$, we also obtain sharp estimates in the cases $X = W^{1,p}(\Omega)$,

$Y = L_p(\Omega)$, $p \in [1, 2]$. For sufficiently smooth domains, almost sharp estimates for the important case $X = W^{2,2}(\Omega)$, $Y = L_2(\Omega)$ are deduced. Corresponding estimates for the parabolic equation are also given. The methodology includes maximum principles, isoperimetric inequalities, special functions and Laplace transformation.

AOR METHODS FOR FINDING THE LEAST SQUARE SOLUTION OF MINIMAL NORM OF RANK DEFICIENT LINEAR SYSTEMS

Hongjiong Tian (*523 Ramapo Valley Road, Mahwah, NJ 07439, USA*)

In this paper we apply AOR methods to find the least square solution of minimal norm to the system $Ay = b$, where A is a complex $m \times n$ matrix with rank r , and b is a complex m -vector. We first augment the system to a block 4×4 consistent system, and then split the augmented matrix by AOR splitting. An interval for the two relaxation parameters where the AOR iteration matrix is convergent is determined. Also, we provide a method to compute the least square solution of minimal norm of the system.

ADAPTIVITY AND A POSTERIORI ERROR ANALYSIS FOR HYPERBOLIC PROBLEMS

P Houston & **E Süli** (*University of Oxford, ICFD, Oxford University Computing Laboratory, Wolfson Building, Parks Road, Oxford OX1 3QD, UK*)

The primary objective of a general adaptive algorithm is to improve the accuracy of a numerical solution by refining the discretisation *locally* in regions where the error is large. In general, an adaptive algorithm will consist of three main components: a local error estimator, a refinement strategy and a stopping condition. The objective of the error estimator is to identify regions in the computational domain where the error is large. Based on this information, the refinement strategy seeks to reduce the error in the computed numerical solution by improving the discretisation locally in these regions. Finally, a stopping criterion must be imposed to prevent refinement *ad infinitum*.

In this paper, we consider each of these components in the context of scalar hyperbolic problems. In particular, emphasis will be given to the construction of reliable *local* error estimators; in this context, by reliable, we mean that the local error estimator gives a good indication of the local error within different regions of the computational domain. Here, we demonstrate that while the norm of the residual of the underlying partial differential equation may be used to bound the error on a global basis, i.e. over the whole computational domain; the norm of the residual, calculated on a small region of the domain (i.e. an element, say), may give a poor estimate of the local error in that region. To reduce this problem, we ‘break-up’ the residual into its different constituent parts. Furthermore, we present some numerical experiments to demonstrate the enhanced reliability of this error indicator.

OPTIMISING COMPUTATIONAL MESHES FOR VARIATIONAL PROBLEMS: A LOCAL APPROACH

F Hülsemann (*University of Bristol, School of Mathematics, University Walk, Bristol BS8 1TW*)

This talk introduces a new approach to mesh optimisation for finite element approximation of variational problems. The novelty of the method lies in its use of data from the immediate neighbourhood of each vertex of the mesh. For a given number of vertices, a mesh is said to be optimal if the finite element approximation obtained on it minimises the

“variational energy functional”. The iterative procedure combines the search for a better nodal position with an update step of the nodal approximation value. This combination of purely local minimisation problems reduces the energy functional monotonically. Numerical results in 2D are obtained using the DIFFPACK library.

SOLUTION PSEUDO ARC LENGTH ERROR CONTROL FOR THE NUMERICAL SOLUTION OF ORDINARY DIFFERENTIAL EQUATIONS

A R Humphries, D J Higham & R Wain (*University of Sussex, School of Mathematical Sciences, Brighton BN1 9QH, UK*)

Standard variable time-stepping algorithms for ODEs are based on the finite time initial value problem paradigm, and consequently admit spurious behaviour in the neighbourhood of fixed points, where there are orbits which are bounded in space but unbounded in time. A new time-stepping strategy is introduced which controls the error in phase space, rather than in time, and essentially bounds the truncation error at each step by a fraction of the solution arc length over the corresponding time-interval. This new error control can be incorporated within a standard algorithm as an additional control at negligible additional computational cost. It will be shown that this new control *prevents* spurious fixed points and period two solutions from arising. In addition the new error control will be shown to be admissible (in the sense that it can always be satisfied with non-zero step-sizes), and to have excellent linear stability properties.

STABILITY OF THE DOUGLAS SPLITTING METHOD

W Hundsdorfer (*CWI, Kruislaan 413, PO Box 94079, 1090 GB Amsterdam, The Netherlands*)

Discretization in space of evolutionary multi-dimensional PDEs leads to large, stiff systems of ODEs $u'(t) = F(t, u(t))$. Often, this F can be decomposed into a number of simpler component functions

$$F(t, w) = F_1(t, w) + F_2(t, w) + \cdots + F_s(t, w).$$

Splitting methods use this decomposition by treating in each stage at most one of the components implicitly. Here we consider the splitting method of Douglas (1962),

$$\begin{aligned} v_0 &= u_n + \tau F(t_n, u_n), \\ v_i &= v_{i-1} + \frac{1}{2}\tau \left(F_i(t_{n+1}, v_i) - F_i(t_n, u_n) \right) \quad (i = 1, 2, \dots, s), \\ u_{n+1} &= v_s, \end{aligned}$$

with step size $\tau = t_{n+1} - t_n$, internal vectors v_i and numerical approximations $u_k \approx u(t_k)$. In this talk some stability results will be presented for scalar, complex test equations, generalizing previous results of Douglas (1962) and of Warming and Beam (1979). The relevance of the theoretical results is discussed for an advection-reaction equation.

ON THE NEW PROPERTIES OF THE FORWARD-JUMPING METHOD FOR SOLVING ODES.

V Ibrahimov (*Baku State University, Department Mathematics of Computation, Faculty Mech. and Mathematics, Republic of Azerbaijan*)

It is known, that one of the effective method for solving initial value problem of the ODEs with the constant coefficients. By the result of G. Dahlquist we receive that, if the k-step

method (explicit or implicit) is stable, then $p \leq 2[k/2] + 2$, here p is the degree and k is the order of the k -step method. We want to note that all the known forward-jumping methods are also subjected to G. Dahlquist's result. Some times ago we constructed the next method

$$y(x+2h) = (8y(x+h) + 11y(x))/19 + h(-f(x+3h, y(x+3h)) + 24f(x+2h, y(x+2h)) + 57f(x+h, y(x+h)) + 10f(x, y(x)))/57$$

($dy/dx = f(x, y)$), which is stable and has the degree $p = 5$. In this case if we don't use forward-jumping method, then for stable method we receive $p \leq 3$ (see G. Dahlquist result). By this way we can construct the stable and A-stable methods with the degree $p = k + m + 1$, where $k \geq 3m$ or $k \geq 3m + 1$ depends from the evenness of k .

Let us consider another method

$$\begin{aligned} y(x+2h) = & (416y(x+h) - 103y(x))/313 + h(157f(x+3h, y(x+3h)) + \dots \\ & 11232f(x+2h, y(x+2h)) + 8451f(x+h, y(x+h)) - \dots \\ & 2830f(x, y(x)))/25353 - h * h(11g(x+3h, y(x+3h)) + \dots \\ & 630g(x+2h, y(x+2h)) - 1557g(x+h, y(x+h)) + \dots \\ & 92g(x, y(x)))/8451 \end{aligned}$$

($df/dx = g(x, y)$).

This method is stable and has the degree $p = 9$. Further we constructed and investigated the forward-jumping multistep multiderivative methods with the constant coefficients in general form.

MULTISTEP METHODS ON MANIFOLDS

A Iserles (*University of Cambridge, Department of Applied Mathematics and Theoretical Physics, UK*)

In this talk we address ourselves to the following question: given an ODE with a solution on a smooth manifold M and a multistep method, can we be assured that the numerical solution will stay on M ? The importance of this question is underscored by the fact that 'staying on the correct manifold' is equivalent to the retention of conservation laws and strong integrals, important qualitative features of the underlying ODE system.

We prove that no multistep method can stay on M whenever the manifold is nonlinear. The main step in our proof is reducing the problem to a question on the geometry of M as a level set, subsequently converting the latter to a problem relating to the Bateman equation.

The outcome of our analysis, together with recent results on Runge–Kutta methods, provide a justification to a quest for new numerical methods with superior qualitative features.

CONTINUOUS SOLUTION OF PLANE PARABOLIC PROBLEM

J Jankowski & J Stefaniak (*Technical University of Poznan, Institute of Applied Mechanics, Piotrowo 3, Poland*)

The fictitious sources method [1] for solving two-dimensional initial-boundary value problem has been applied. As an example the temperature in a rectangular plate with the

mixed boundary conditions has been found. The boundary conditions are prescribed functions of time. The obtained continuous, approximate solution of that problem has been compared with the given boundary conditions.

[1] J.Stefaniak, The Method of Concentrated Sources in Heat Conduction, Journal of Thermal Stresses, 19 :481-493, 1996

A NON-CONFORMING ADAPTIVE FEM FOR STOKES' PROBLEM

S Jansche & C Carstensen (*Christian-Albrechts-Universitaet, Mathematisches Seminar, Ludewig-Meyn-Str. 4, D-24098 Kiel, Germany*)

A computable reliable and efficient error estimate is established for the Stokes problem. The proof is based on a Helmholtz decomposition and inverse estimate techniques. This justifies an adaptive mesh refinement algorithm for (non-conform) Crouzeix-Raviart Elements. Numerical experiments clearly indicate the superiority of the proposed scheme.

SOME A POSTERIORI ERROR ESTIMATORS FOR THE STOKES PROBLEM

D Kay & D Silvester (*UMIST, Department of Mathematics, PO BOX 88, Manchester M60 1QD, UK*)

Three different types of a posteriori error estimators are considered for the locally stabilised element P_1-P_0 . The first is given by a norm of the residual, the second is obtained from the solution of local Stokes problems, and the third is obtained from the solution of local Poisson problems. All three estimators are shown to be equivalent to the true error independently of the choice of stabilisation parameter.

An adaptive mesh refinement technique is given that creates meshes that conform to the requirements of the local stabilisation.

Some numerical results show that the estimators provide reasonable approximations to the true error. They also show that the estimators are good at detecting local singularities in the true solution.

A PARALLEL COLLOCATION METHOD FOR TWO DIMENSIONAL LINEAR SEPARABLE PARABOLIC DIFFERENTIAL EQUATIONS

P Keast & Y Wang (*Dalhousie University, Department of Mathematics, Statistics and Computer Science, Halifax, Canada*)

If the method of lines approach is taken in the numerical solution of linear separable parabolic equations in two or more space variables, systems of ordinary differential equations arise which may be decoupled by means of a matrix decomposition technique. The resulting systems can be solved efficiently in parallel using a reliable initial value ODE solver, and the solution recovered. Experimental software to implement this procedure has been constructed, based on B-splines, a special linear equation solver to take advantage of the structure of the linear systems, a generalized eigenvalue routine from Eispack, and DASSL to solve the ODEs. The method performs well in a parallel environment.

BACKWARD ERROR IN THE POWER METHOD

P A Knight (*University of Strathclyde, Department of Mathematics, Glasgow, G1 1XH, UK*)

The Power Method is probably the simplest numerical method for computing eigenvalues that one encounters. Despite this simplicity, there are few published results concerning its behaviour when subjected to rounding errors. It is known that in certain situations the Power Method can have large backward errors. We explain why this is to be expected if the matrix is sufficiently nonnormal. We also derive conditions that can guarantee backward stability in the algorithm, and present numerical evidence that these conditions can be extended to include a wide class of matrices.

In order to motivate and prove our results we view the Power Method as a dynamical system. This also allows us to establish an interesting result connecting the speed of convergence to nonnormality. We conclude by suggesting future directions for our research.

ϵ -ENTROPY OF SOBOLEV'S CLASSES ON S^d

A Kushpel, J Levesley & K Tas (*MECC-UNICAMP, CAIXA Postal 6065,13081-970 Campinas SP, Brazil*)

Let X be a Banach space and $A \subset X$ be compact. For a fixed $\epsilon > 0$ a finite set of points $x_1, \dots, x_n$ is called an ϵ -net for A if for each $x \in A$ there is at least one point x_k of the net at a distance from x not exceeding ϵ . The logarithm $H_\epsilon(A) = \log N_\epsilon(A)$, where $N_\epsilon(A) := \min\{n : \{x_1, \dots, x_n\} \in A \text{ is an } \epsilon \text{ net}\}$, is the entropy of the set A .

The last thirty years have seen an explosion of interest in ϵ -entropy and related topics. We just mention here contributions of Carl, Edmunds, Kolmogorov, Mitjagin, Pietch, Tikhomirov, Triebel, to name but a few.

Sharp orders of ϵ -entropy of classical Sobolev's classes $W_p^\alpha(S^d)$ in $L_q(S^d)$ are established for all $1 \leq p, q \leq \infty$. The analysis is essentially based on some results from the geometry of finite dimensional convex bodies.

Let R^d be a d -dimensional Euclidean space with usual scalar product $\langle x, y \rangle = \sum_{k=1}^d x_k y_k$ and S^d be the d -dimensional unit sphere in R^{d+1} . Let $H_k = \{f | \Delta f = \gamma_k f\}$ be an eigenspace of the Laplace-Beltrami operator Δ for the sphere corresponding to the eigenvalue $\gamma_k = -k(d+k-1)$ and $Z_\eta^{(k)}(x)$ is a real unique zonal (i.e. invariant under the action of all the rotations of S^d which fix η) element of H_k . Let $d\mu$ be a rotation invariant normalised measure on S^d and $L_p(S^d)$, $1 \leq p \leq \infty$ be the usual space of p -integrable functions on S^d . For any $\alpha > 0$ and $1 \leq p \leq \infty$ the classical Sobolev classes on a sphere are defined as usual:

$$W_p^\alpha(S^d) = \{f(x) | f(x) = \int_{S^d} g_\alpha(\langle x, y \rangle) \varphi(y) d\mu(y), \| \varphi \|_p \leq 1, \int_{S^d} \varphi(x) d\mu = 0, \}.$$

where $g_{\alpha, \eta}(x) \sim \sum_{k=1}^\infty (k(k+d-1))^{-\frac{\alpha}{2}} Z_\eta^{(k)}(x)$.

For the ease of notation we will write $a_n \ll b_n$ for two sequences, if $a_n \leq cb_n$ for $n \in N$ and $a_n \asymp b_n$, if $c_1 b_n \leq a_n \leq c_2 b_n$ for all $n \in N$ and some constants c , c_1 and c_2 .

The main result which will be discussed is

Theorem

For the Sobolev classes on S^d , $d \geq 2$ we have the following weak asymptotics:

$$H_\epsilon(W_p^\alpha(S^d), L_q(S^d)) \asymp \epsilon^{-\frac{d}{\alpha}}, \quad \epsilon \rightarrow \infty,$$

where $\alpha > d$ and $1 \leq p, q \leq \infty$.

CONVERGENCE RESULTS FOR THE MATLAB ODE23 ROUTINE

H Lamba & A M Stuart (*Stanford University, Division of Mechanics and Computation, California 94305-4040, USA*)

We prove convergence results on finite time intervals, as the user-defined tolerance $\tau \rightarrow 0$, for a class of adaptive time-stepping ODE solvers that includes the MATLAB ode23 routine. In contrast to existing theories, these convergence results hold with error constants that are uniform in the neighbourhood of equilibria; such uniformity is crucial for the derivation of results concerning the numerical approximation of dynamical systems. For linear problems the error estimates are uniform on compact sets of initial data. The analysis relies upon the identification of explicit embedded Runge-Kutta pairs for which all but the leading order terms of the expansion of the local error estimate are $\mathcal{O}(\|f(u)\|^2)$.

DOMAIN EMBEDDING BOUNDARY INTEGRAL METHODS AND PARABOLIC PDES

S Langdon (*University of Bath, School of Mathematical Sciences, Bath BA2 7AY, UK*)

The classical applications of boundary integral equation (BIE) methods are often to boundary value problems for homogeneous PDEs, where one is interested in computing the complementary Cauchy data for the problem. Both inhomogeneous PDEs and/or problems where one is interested in the solution throughout a domain are sometimes considered less appropriate for BIE treatment, because of the cost of computing particular solutions to remove the inhomogeneity and/or the cost of many field point evaluations.

An approach which allows the solution of both these problems in a single framework is the domain embedding approach of Mayo, Greengard et.al.. This consists of embedding the domain, on which we seek a solution, in a fictitious domain (rectangular in two dimensions) on which finite differences fit nicely. Here we discuss this approach when the actual domain of interest has a smooth but possibly complicated boundary.

Solving an extended problem on the rectangular domain gives a particular solution to the inhomogeneous problem. One can then solve the corresponding homogeneous problem on the smooth domain by a boundary integral method. The problem of making many field point evaluations can be overcome by evaluating the solution directly at only a small number of carefully chosen mesh points near the boundary of the smooth domain. This is done using Taylor series expansions of the solution about nearby points on the boundary, with the coefficients computed by a “bootstrapping” technique, thus avoiding the computation of nearly singular integrals. One can then use a fast solver to extend the solution to the rest of the domain.

This idea could be used to solve parabolic problems on smooth irregular domains, where linearly implicit timestepping reduces the problem to a sequence of Helmholtz problems, each of which can be solved in this way.

THE NORM OF THE FOURIER PROJECTION IN WEIGHTED L_p SPACES

J Levesley & A K Kushpel (*University of Leicester, Dept. of Maths and Comp. Science, Leicester, LE1 7RH, UK*)

It is well known that the Chebyshev series for a function in L_p converges in L_p if $1 < p < \infty$, and that for $p = 1$ or ∞ the norm of the projection behaves like $\log n$. In two papers Pollard shows that the Fourier projection for Gegenbauer polynomials with index λ converges in L_p if $(2\lambda + 1)/(\lambda + 1) < p < (2\lambda + 1)/\lambda$. We give estimates for the growth of the norm of the projection when p is not in the range of convergence.

NONLINEAR PROGRAMMING WITHOUT A PENALTY FUNCTION

S Leyffer & R Fletcher (*University of Dundee, Department of Mathematics and Computer Science, Dundee DD1 4HN, UK*)

In this talk the solution of nonlinear programming problems by a Sequential Quadratic Programming (SQP) trust-region algorithm is considered. The aim of the present work is to promote global convergence without the need to use a penalty function. Instead, a new concept of a “filter” is introduced which allows a step to be accepted if it reduces *either* the objective function *or* the constraint violation function. Numerical tests on a wide range of test problems are very encouraging and the new algorithm compares favourably with LANCELOT and an implementation of Sl_1QP .

SUPERCONVERGENCE OF COUPLING TECHNIQUES IN COMBINED METHODS FOR ELLIPTIC EQUATIONS WITH SINGULARITIES

Zi-Cai Li (*National Sun Yat-sen University, Department of Applied Mathematics, Kaohsiung 80424, Taiwan*)

Different coupling techniques, such as the nonconforming constraints, penalty and hybrid integrals, of the Ritz-Galerkin and finite difference methods are presented for solving elliptic boundary value problems with singularities. Based on suitable norms involving discrete solutions at specific points, superconvergence rates on solution derivatives are exploited by using five combinations, e.g., the nonconforming combination, the penalty combination, Combinations I and II, and Symmetric combination. For quasiuniform rectangular difference grids, the superconvergence rates, $O(h^{2-\delta})$, of solution derivatives by all five combinations can be achieved, where h is the maximal mesh length of difference grids used in the finite difference method, and $\delta(> 0)$ is an arbitrarily small number.

Emphasis on superconvergence analysis in this paper lies in estimates on error bounds caused by the coupling techniques and their incorporation with the finite difference method used. Therefore, the similar analysis and conclusions may be extended to linear finite element methods using triangulation by referring the existing references. Moreover, the simplest penalty combination having $O(h^{2-\delta})$ of solution derivatives is well suited to solving the engineering problems with multiple singularities and multiple interfaces.

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THE STREAMLINE DIFFUSION FEM ON SHISHKIN MESHES FOR CONVECTION-DIFFUSION PROBLEMS

T Linß & M Stynes (*University College Cork, Department of Mathematics, Republic of Ireland*)

We consider singularly perturbed linear elliptic problems in two dimensions. The solutions of such problems typically exhibit layers and are difficult to solve numerically. The streamline diffusion method has been proven to produce accurate solutions away from any layers on uniform meshes, but fails to compute the boundary layers precisely. Our modified SDFEM incorporates Shishkin meshes to resolve boundary layers. We give numerical results and local L_∞ error estimates that are uniform with respect to the perturbation parameter.

PRECONDITIONERS FOR CONVECTION-DIFFUSION PROBLEMS

D Loghin (*University of Oxford, Computing Laboratory, Wolfson Building, Parks Road, Oxford OX1 3QD, UK*)

Although the Green's function associated with the convection-diffusion operator is generally not available, some of its properties (directionality and radial symmetry) are sufficient to suggest a class of efficient preconditioners. Being based on the Green's function we expect them to perform well on suitable discretizations, be they arising from a SUPG or simply a standard Galerkin formulation with mesh Peclet number less than 2. Convergence independent of the mesh is proved for fixed wind direction convection dominated problems on the unit square.

HOMOCLINIC ORBITS AND LOCALIZED BUCKLING OF AXIALLY-COMPRESSED CYLINDRICAL SHELLS

G J Lord (*University of Bristol, Department of Engineering Maths, Bristol, BS8 1TR, UK*)

The buckling of a long elastic cylindrical shell under axial compression is a classical problem in structural mechanics. The most widely used model to describe the buckling phenomena is given by the von Karman-Donnell equations. It has long been observed experimentally that the buckling occurs locally on axial length of the cylinder. A standard analytic approach adopted by Koiter and others is that the pattern comprises of an interaction of eigen modes which are periodic both axially and circumferentially. The equations do indeed admit such solutions and until recently localization was presumed to occur from imperfections. However in 1991 Hunt & Lucena Neto showed the existence of axially localized solutions through asymptotic analysis.

In this talk we consider an infinitely long cylinder and introduce the von Karman-Donnell equations. We discretize these equations by a Galerkin approximation in the circumferential direction. We describe an adaptation of standard methods for the location and parameter continuation of homoclinic solutions making special use of the symmetry and reversibility properties of solutions observed experimentally.

These methods are illustrated numerically and a variety of homoclinic solutions of the equations are computed along with their bifurcation diagrams as load varies. All computations are performed using AUTO. The techniques illustrated here for the von Karman-Donnell equations are applicable to a wider class of PDEs.

INTEGRATION RULES OF SPECIFIED TRIGONOMETRIC DEGREE

J Lyness (*Argonne National Laboratory, Mathematics and Computer Science Div., Argonne, Illinois 60439, USA*)

The general theory of numerical integration over a hypercube of a periodic function is not well known. In this talk, the roles of lattice rules, merit rules and the reproducing kernel are mentioned, and some recently discovered integration rules are reported.

NUMERICAL SOLUTION OF THE FLOW OF WET STEAM IN A STEAM TURBINE USING AN EULERIAN CODE

M McCallum & R Hunt (*University of Strathclyde, Department of Mathematics, Glasgow, G1 1XH, UK*)

The formation of water droplets in a low pressure steam turbine seriously degrades the efficiency of the generator. A model has been developed which includes the nucleation and subsequent growth of the droplets as the extra equations to the usual Euler equations for dry steam. A feature of this work is that all the equations are cast in Eulerian form compared to much of the previous work which looked at a Lagrangian form. The ensuing equations are solved using a second order upwind TVD scheme which can cope with the steep gradients which can occur in the solution. The results for a 1-D nozzle will be presented and compared with experimental results and preliminary results for the 2-D flow through a cascade of turbine blades will also be given.

This work is supported by EPSRC and GEC-Alsthom Turbine Generators Ltd.

CONVERGENCE ANALYSIS OF FINITE-DIFFERENCE APPROXIMATIONS OF AN INHOMOGENEOUS SINGULARLY PERTURBED BOUNDARY VALUE PROBLEM USING GRID EQUIDISTRIBUTION

J A Mackenzie & G Beckett (*University of Strathclyde, Department of Mathematics, Glasgow G1 1XH, UK*)

We derive ϵ -uniform error estimates for two first-order upwind discretisations of a model inhomogeneous, second-order, singularly perturbed boundary value problem on a non-uniform grid. Here, ϵ is the small parameter multiplying the highest derivative term. The grid is suggested by the equidistribution of a positive monitor function which is a linear combination of a constant floor and a power of the second derivative of the solution. Analysis shows how the floor should be chosen to ensure ϵ -uniform convergence. The use of equidistribution principles appears in many grid adaption schemes and our analysis indicates the convergence behaviour on such grids. Numerical results are given that confirm the analysis.

NUMERICAL SOLUTION OF THE ORR-SOMMERFELD EQUATION BY THE FEM ON A SHISHKIN MESH

N Madden & M Stynes (*University College Cork, Department of Mathematics, Ireland*)

Klopman's model for wave-current interactions leads to the Orr-Sommerfeld equation of classical hydrodynamic stability, but here the presence of an extra parameter makes the problem nonlinear. The solution to this fourth-order, complex-valued ODE will have layers at both ends of the domain because of the small viscosity term. An accurate solution within these layers is required in the model for the computation of the wave-number and the bed stresses. A finite element method on a Shishkin mesh is used and the results are shown to compare favourably with the results of other researchers.

VARIABLE TRANSFORMATIONS IN THE NUMERICAL SOLUTION OF SECOND KIND VOLTERRA INTEGRAL EQUATIONS

A Makroglou (*University of Portsmouth, School of Computer Science and Mathematics, Portsmouth PO1 2EG, UK*)

A number of techniques which use variable transformations in numerical integration have been developed recently. The use of these transformations resulted in increasing the order of convergence of the trapezoidal rule. In this presentation the application of variable transformation techniques to the numerical solution of second kind Volterra integral equations will be considered.

THE IDENTIFICATION OF SPURIOUS SOLUTIONS GENERATED BY NUMERICAL SOLUTION TECHNIQUES, USING A DISCRETE MULTIPLE SCALES ANALYSIS

E Maré & S W Schoombie (*University of the Orange Free State, P. O. Box 339, Bloemfontein 9300, South Africa*)

In this contribution we illustrate the use of a discrete multiple scales analysis technique to identify spurious solutions of generalized finite difference approximations to the Korteweg-de Vries equation.

Of particular interest is the behaviour of spurious solutions as the finite difference grid length parameter tends to zero. We also illustrate the behaviour of spurious solutions as the order of the finite difference approximation is increased.

NUMERICAL SOLUTION OF SINGULAR BOUNDARY VALUE AND EIGENVALUE PROBLEMS FOR SELFADJOINT DIFFERENTIAL OPERATORS

M. Marletta (*University of Leicester, Department of Mathematics and Computer Science, UK*)

The classical technique for solving singular boundary value problems involves a regularisation, usually achieved by truncating the interval to avoid the singular endpoint. Artificial boundary conditions must then be imposed at the truncated end. Classical work was done on these problems in the late seventies by Lentini and Keller.

In this talk we restrict our attention to **selfadjoint** differential operators of arbitrary even order. We show that the Von Neumann formula for the domain of a selfadjoint operator suggests at least some of the artificial boundary conditions which should be imposed. We construct the remaining boundary conditions to ensure a ‘spectrally exact’ approximation of the original singular operator. A significant feature is that this approach requires much less information about asymptotic behaviour of the solutions of the differential equations near the singular endpoint: in fact, the only information required is that obtained from the Von Neumann decomposition.

PRIMAL AND M-H MODELS OF UNSATURATED POROUS MEDIA FLOW

J Maryška, D Frydrych & V Wasserbauer (*TU Liberec, Hálkova 6, 461 17 Liberec, Czech Republic*)

The mathematical model of steady unsaturated porous media flow is discussed. A compact expression of the governing equations is found and an existence theorem for the primal formulation is proved. The iterative scheme for solution of this nonlinear problem is proposed and the computational results are compared with real data and free-boundary approach.

EMPLOYMENT OF RECENT PHDs: HOW THE CULTURE IS CHANGING IN HIGHER EDUCATION

J L Mead (*Arizona State University, Department of Mathematics, Tempe, AZ 85287-1804, USA*)

Employment in the early post-Ph.D years is crucial to career development. As the climate in higher education changes, jobs are more difficult to secure. As a Ph.D student at Arizona State University, I have been participating in the Preparing Future Faculty program, a national program originally funded by the Pew Charitable Trusts and the

American Association of Colleges and Universities and now institutionalized at ASU. We discuss topics such as publishing, funding opportunities, applying for jobs, interviewing for positions, and faculty roles at different higher educational settings with college and university faculty and administrators. A brief presentation will be made on these topics in order to begin a group discussion on careers for Ph.Ds.

ANALYSIS OF A PIVOTING STRATEGY FOR GAUSSIAN ELIMINATION IN PARALLEL

J L Mead (*Arizona State University, Department of Mathematics, Tempe, AZ 85287-1804, USA*)

A pivoting strategy was introduced by Onaga and Takechi to improve Gaussian elimination with partial pivoting on parallel machines. This method is cheaper on parallel machines because one row transport is eliminated per pivoting step when rows are added instead of pivoted. It is shown that this pivoting strategy results in growth bounded above by $3^{(N-1)}$ rather than $2^{(N-1)}$ in the usual case. Growth factors near this bound are found for near singular matrices where the growth is small for the usual pivoting strategy. Numerical results verify this algorithm may fail when partial pivoting is stable even though for the average case, the two methods are comparable.

PARALLEL LINEAR SYSTEM SOLVERS FOR RUNGE-KUTTA-NYSTRÖM METHODS

E Messina & P J van der Houwen (*University of Naples 'Federico II', Dipartimento di Matematica e Applicazioni, via Cintia, I-80126 Naples, Italy*)

Solving the nonlinear equations arising in implicit Runge-Kutta-Nyström type methods by (modified) Newton iterations leads to linear systems whose matrix of coefficients is of the form $I - A \otimes h^2 J$ where A is the Runge-Kutta-Nyström matrix and J an approximation to the Jacobian of the righthand side function of the system of differential equations. For larger systems of differential equations, the solution of these linear systems by a direct linear solver is very costly, mainly because of the LU-decompositions. We try to reduce these costs by solving the linear Newton systems by an inner iteration process. Each inner iteration again requires the solution of a linear system. However, the matrix of coefficients in these new linear systems are of the form $I - B \otimes h^2 J$ where B is a nondefective matrix with positive eigenvalues, so that by a similarity transformation, we can decouple the system into subsystems the dimension of which equals the dimension of the system of differential equations. Since the subsystems can be solved in parallel, the resulting integration method is highly efficient on parallel computer systems. The performance of the Parallel Iterative Linear System method for Runge-Kutta-Nyström equations (PILSRKN method) will be illustrated by means of a few examples from the literature.

NUMERICAL SOLUTION OF A CONSTRAINED 2-DIMENSIONAL GUILLOTINE CUTTING PROBLEM

R Middleton (*University of Dundee, Department of Mathematics and Computer Science, Dundee DD1 4HN, UK*)

The constrained 2-d stock cutting problem seeks an optimal cutting pattern that cuts a given set of rectangles from standard stock sheets with minimum waste. Problems of this type are very hard combinatorial problems and traditionally heuristic methods are employed. A new MINL formulation is presented and a method of solution is described.

The specific problem to be solved describes an application from the glass cutting industry.

EVOLUTION-GALERKIN SCHEMES FOR HYPERBOLIC EQUATIONS

K W Morton (*University of Oxford, Computing Laboratory, Oxford OX1 3QD, UK*)

The PERU, evolution-Galerkin, or evolution-projection schema provides a valuable framework for devising, analysing and comparing alternative approximations to hyperbolic PDE's. The second order wave equation is an important model problem; and there has been renewed interest in the bicharacteristic-based schemes devised by D. S. Butler (1960).

We will emphasise the need for third order accurate schemes and show how they can be developed.

MIXED-HYBRID MODEL OF UNSTEADY FREE BOUNDARY POROUS MEDIA FLOW FLUID

J Muřák, D Frydrych & J Maryřka (*DIAMO, Mathematical Modelling Department, DIAMO, s.e., 471 27 Stráž pod Ralskem, Czech Republic*)

The mixed-hybrid model of unsteady porous media flow is studied. The free boundary problem arising in each time step of Rothe method is treated by a shape optimization approach and the existence of solution on each time level is proved.

DEFECT CORRECTION AND DOMAIN DECOMPOSITION FOR SECOND ORDER BOUNDARY VALUE PROBLEMS

K Nafa (*University of Annaba, Institute of Mathematics, BP 12, Annaba 23000, Algeria*)

A STUDY OF A MODEL PROBLEM IN ELECTRO-PHYSIOLOGY BY A SPECTRAL METHOD

F Z Nouri (*University of Annaba, Institut De Mathematiques Universite De Annaba BP12, Annaba 23000, Algeria*)

The purpose of this paper is to numerically simulate the potential diffusion inside a neuron of a vertebrate central nervous system, under the action of suitable external stimulations. Information about the electric conduction properties of the neuron is provided by W. Rall. The spectral collocation at the Legendre Gauss-Lobatto nodes is used.

EFFICIENT METHODS USING HIGH ACCURACY APPROXIMATE INERTIAL MANIFOLDS

J Novo & E S Titi (*Universidad de Valladolid, Dpto Matematica Aplicada y Computacion, Facultad de Ciencias, 47011 Valladolid, Spain*)

In [1] a computationally inexpensive postprocessing of Fourier Spectral or Pseudospectral methods for the discretization of dissipative equations was introduced. The postprocessed Galerkin method uses the same approximate inertial manifold ($\Phi_{app} = \Phi_1$) (see [2]) as the Nonlinear Galerkin methods (NLG) [3] and obtains the same convergence rates. This is done at virtually no extra computational cost, so that the Postprocessed method is more efficient than both Galerkin and NLG methods. The results on [1] are only valid for Φ_1 (not for more accurate inertial manifolds) but the possibility of complementing the Galerkin or Pseudospectral methods with more accurate inertial manifolds remains open.

Here, a postprocess of the Postprocessed Galerkin or Pseudospectral method that appears in [1] is presented. We also study a postprocess of the Nonlinear Galerkin method. Both

methods use the same approximate inertial manifold $\Phi_{app} = \Phi_2$ that appears for example in [4] and [5] (a more accurate manifold than Φ_1).

The order of convergence of the two Φ_2 -Postprocessed methods for a representative class of equations is the same and improves the order of convergence of the Postprocessed Galerkin or Pseudospectral method or the NLG method respectively. This is proved for some problems in one and two spatial dimensions including the Navier-Stokes equations under periodic boundary conditions or homeogeneous (nonslip) Dirichlet boundary conditions.

Numerical experiments will show that this postprocess makes the Φ_2 -Postprocessed Galerkin or Pseudospectral method much more efficient than the Φ_1 one presented in [1]. And the Φ_2 -Postprocessed NLG more efficient than the NLG (that uses the Φ_1 approximate inertial manifold).

[1] B. García-Archilla, J. Novo and E.S. Titi, Postprocessing the Galerkin method: A novel approach to Approximate inertial manifolds, *SIAM J. Numer. Anal.*, (to appear).

[2] C. Foias, O. Manley and R. Temam, Modelling of the interaction of small and large eddies in two dimensional turbulent flows, *Math. Mod. Num. Anal.*, M²AN, 22, 1988, 93-114.

[3] M. Marion and R. Temam, Nonlinear Galerkin Methods, *SIAM J. Numer. Anal.*, 26, 1989, 1139-1157.

[4] C. Devulder, M. Marion and E.S. Titi, On the rate of convergence of the nonlinear Galerkin methods, *Math. Compt.*, 60, 1993, 495-514.

[5] A. Debussche and M. Marion, On the construction of families of approximate interial manifolds, *J. Diff. Eq.*, 100, 1992, 173-201.

ON POSITIVE QUINTIC POLYNOMIALS

G Opfer (*University of Hamburg, Institute of Applied Mathematics, Bundesstr. 55, D-20146 Hamburg, Germany*)

Let there be a polynomial p of degree n defined on a (compact, nontrivial) interval $I := [a, b]$. The general question is how to decide whether the polynomial p is nonnegative throughout I just by looking at the coefficients (in a certain basis) or by looking at $n + 1$ values and derivatives at the endpoints or by looking at some other relevant data compiled from the polynomial. If $n = 0$ the answer is trivial: $p \geq 0$ if and only if $p(a) \geq 0$, similarly for $n = 1$: $p \geq 0$ if and only if $p(a) \geq 0$ and $p(b) \geq 0$. For quadratic polynomials the answer is already a little more complicated. It seems that the literature stops with quartic polynomials (G. Ulrich, L.T. Watson, *SIAM J. Sci. Comput.* 15(1994), 528-544). When searching for nonnegative quintic splines (together with H. J. Oberle, to appear in *Numer. Math.*) we found some (endpoint) conditions for quintic polynomials which leave them nonnegative. The talk will be on this topic.

SCHWARZ METHODS FOR A SINGULARLY PERTURBED SELF-ADJOINT PROBLEM

E O’Riordan, J J H Miller & G I Shishkin (*Dublin City University, School of Mathematical Sciences, Dublin, Ireland*)

In this paper a singularly perturbed self-adjoint ordinary differential equation is examined. It is shown that a suitably designed Schwarz method which uses a standard finite difference operator on uniform meshes gives approximations which converge in the max-

imum norm to the exact solution, independently of the singular perturbation parameter. The convergence rate is shown to be essentially second order uniformly with respect to the singular perturbation parameter.

CYCLIC REDUCTION, DICHOTOMY, AND THE ESTIMATION OF DIFFERENTIAL EQUATIONS

M R Osborne (*Australian National University, School of Mathematical Sciences, Canberra, ACT 0200, Australia*)

In the estimation of ordinary differential equations given observed data it is necessary to parametrize the solutions of the differential equations in a computationally tractable manner in order to facilitate comparisons with the observed data. Typically this is done by adjoining initial or boundary conditions to the differential system in order to completely specify these comparison solutions. This requires additional information such as the dichotomy structure of the problem in order to do this in a manner that guarantees stable computations. Here, cyclic reduction is used to reduce the estimation problem to an optimization problem subject to a fixed number of equality constraints. If orthogonal transformations are used in the cyclic reduction process then it appears that stable computations are possible without the need for the structural information needed to devise the stable imbeddings. The process produces a new family of representations of the solutions of the ODE system, and this is described.

A FINITE ELEMENT SOLUTION IN 3D FOR THE UNSTEADY CONVECTION-DIFFUSION EQUATION

S Osmani (*University of Tirana, Faculty of Geology and Mining, Tirana, Albania*)

This paper presents a Finite Element Solution for the unsteady Convection-Diffusion Equation in three space dimensions. The integration of the equation is based on Galerkin's principle. According to this method and using a three-linear base has been obtained a differential system. By applying a finite difference scheme this one has been transformed into an algebraic equations system, by which is obtained the solution. Basing on the above algorithm are presented some simple examples from reservoir engineering.

Finally, the three-linear base used in this algorithm improves the accuracy of solution.

THE ERROR OF THE CRANK-NICOLSON METHOD FOR LINEAR PARABOLIC EQUATIONS WITH A DERIVATIVE BOUNDARY CONDITION

O Østerby (*Aarhus University, Computer Science Department, DK 8000 Aarhus C, Denmark*)

The accuracy of finite difference formulae for partial differential equations is usually characterized by the approximation order of the local truncation error as determined by Taylor expansions. Thus the local truncation error of the Crank-Nicolson formula is second order in the two step sizes, h and k , and this carries over to the global error in case of Dirichlet boundary conditions, but not if a derivative boundary condition is approximated by a first order formula. We study the pointwise global error on the form

$$hc(t, x) + kd(t, x) + h^2f(t, x) + k^2g(t, x) + \dots$$

and show that the auxiliary functions c , d , f and g are solutions to related parabolic problems. We also present a method based on the computed numbers on refined grids

to determine the order of the error and the dominant terms in the error expansion. The techniques are demonstrated on two examples.

LONG TIME ERROR BOUNDS FOR THE DISCRETIZATIONS OF NONAUTONOMOUS PARABOLIC PROBLEMS: THE METHOD OF SHADOWING

C Palencia & A Ostermann (*Universidad de Valladolid, Dpto Matematica Aplicada y Computacion, Facultad de Ciencias, 47011 Valladolid, Spain*)

Discretizations in time of nonautonomous parabolic problems based on Runge–Kutta methods are considered. The method of shadowing is used to derive estimates depending only the relative total variation of the coefficients of the parabolic problems, in independence of the length of the time interval considered. We do not assume the existence of a dichotomy for the continuous and the discrete problems in common. Due to some regularity requirements, at the end the scope is restricted to the backward Euler method.

INTERPOLATION OF DATA GIVEN AT FUZZY NODES

M Parsaei (*University of Tehran, Department of Mathematics and Computer Science, Iran*)

The subject of uncertainty in data values can play an important role in real physical problems. In interpolation of functions this can be in the form of uncertainties in the given function values or inexactness in the position in which the function values are given. Lowen {Fuzzy Sets and Systems 34(1990) 33-38} and Kaleva {Fuzzy Sets and Systems 61(1994) 63-70} have applied fuzziness to the value of the functions. In this talk we will fuzzify the positions in which (exact) values of the function is given, using Lagrange interpolation this means that the Lagrange coefficients will be fuzzy functions and can not be considered as crisp basis functions. we will use L-L type fuzzy numbers and demonstrate that in a simplified case the membership function of the resulting interpolation polynomial can be presented in triangular form. Some numerical results will be presented.

PREASSIGNED ABSCISSAE AND HYBRID QUADRATURES

T N L Patterson (*The Queen's University of Belfast, Department of Applied Mathematics & Theoretical Physics, Belfast, N. Ireland, BT7 1NN , UK*)

A generalisation of stratified nested quadrature is discussed leading to hybrid rules which combine the properties of stratification with highest possible precision.

A FAST TWO-GRID METHOD FOR A ROUGH SURFACE SCATTERING PROBLEM

M Rahman, S N Chandler-Wilde & C R Ross (*Brunel University, Department of Mathematics and Statistics, Uxbridge, UB8 3PH, UK*)

We consider a model problem of one-dimensional rough surface scattering, in which a plane wave is incident upon a flat boundary on which the total field satisfies an impedance boundary condition with arbitrary inhomogeneous surface impedance.

Using a novel radiation condition the problem is formulated as a uniquely solvable second kind boundary integral equation on the whole real line (the infinite boundary). To solve the integral equation approximately the range of integration is truncated to the finite interval $[-A, A]$. We show that the resulting approximate solution converges to the true

solution locally, and present error estimates which depend on the position of the field point and A .

Next we discuss discretisation of the problem and establish an error estimate for a simple piecewise constant boundary element method on a uniform mesh, that the discretisation error is bounded by $Ckh \log(kh)$, where k is the wavenumber, h the stepsize, and C an absolute constant. (To the authors' knowledge this is the first time that an error estimate with a constant independent of the wavenumber has been obtained for the boundary element solution of a wave scattering problem.)

To obtain accurate results with these methods kh must be small and kA large, leading to a large full linear system of order N . We show numerical results and present numerical analysis for a fast iterative solution scheme. This scheme uses a simple two-grid (multigrid) method and carries out the required matrix vector multiplications efficiently using the FFT (the integral operator is the product of a multiplication and a convolution). Results correct to discretisation error are achieved in $O(N \log N)$ computations.

TOWARDS PARAMETER-FREE STREAMLINE UPWINDING FOR ADVECTION-DIFFUSION PROBLEMS

A Ramage, B Fischer, D Silvester & A Wathen (*University of Strathclyde, Department of Mathematics, Glasgow G1 1XH, UK*)

We consider the design of robust and efficient finite element approximation methods for solving advection-diffusion equations. Specifically, we examine the stabilisation of discrete approximations using uniform grids which do not resolve boundary layers, as might arise using a multi-level (or multigrid) iteration strategy. In particular, we show that when using SUPG (streamline-upwind) finite element methodology, there is a symbiotic relationship between 'optimal' solution approximation and fast convergence of smoothers based on the standard GMRES iteration.

A STEEPEST-EDGE SIMPLEX CODE FOR LARGE LINEAR PROGRAMS

J Reid (*Rutherford Appleton Laboratory, Didcot OX11 0QX, UK*)

It is over 20 years since I wrote the Harwell Subroutine Library Fortran package LA05 for handling linear programming basis matrices. This factorizes the matrix using threshold pivoting with Markowitz' sparsity strategy and updates the factorization after each simplex step using a variant of the Golub-Bartels strategy that preserves sparsity better. This code has been widely used in a variety of LP codes.

I tested LA05 in the framework on a steepest-edge code LA04 that I intended to put in the Harwell Subroutine Library. To my shame, I have allowed this to gather dust uncompleted. A recent request has prompted me to work on this afresh. It contains a number of novel strategies for ensuring robustness and is able to solve efficiently all the Netlib test problems except for DFL001, QAP12, and QAP15, each of which is very large and recognized as particularly difficult.

In this talk, I will explain the strategies for ensuring robustness, present some performance statistics on the Netlib set, and report on work in progress on improvements to address the difficulties exposed by the remaining three test problems.

A PARALLEL MULTISPLITTING SOLUTION OF THE LEAST SQUARES PROBLEM

R A Renaut (*Arizona State University, Dept. of Mathematics, Tempe, AZ 85287-1804, USA*)

The linear least squares problem, $\min_x \|Ax - b\|_2$, is solved by applying a multisplitting (MS) strategy in which the system matrix is decomposed by columns into p blocks. The b and x vectors are partitioned consistently with the matrix decomposition. The global least squares problem is then replaced by a sequence of local least squares problems which can be solved in parallel by MS. In MS the solutions to the local problems are recombined using weighting matrices to pick out the appropriate components of each subproblem solution. A new two-stage algorithm which optimizes the global update each iteration is also given. For this algorithm the updates are obtained by finding the optimal update with respect to the weights of the recombination. For the least squares problem presented the global update optimization can also be formulated as a least squares problem of dimension p . Theoretical results are presented which prove the convergence of the iterations. Numerical results which detail the iteration behavior relative to subproblem size, convergence criteria and recombination techniques are given. The two-stage MS strategy is shown to be effective for near-separable problems.

SPLIT-STEP METHODS FOR QUANTUM PROBLEMS

M A Revilla, J de Frutos & N Reguera (*Universidad de Valladolid, Departamento de Matematica Aplicada y Computacion, Spain*)

In [1], the authors calculate numerically populations of excited vibrational states and dissociation probabilities for the interaction of a Morse oscillator with a chirped, ultrashort, intense laser pulse. They use a split second order method with a very small time step.

Here, we use higher order split integrators as well as the alternative technique suggested in [2], and compare the efficiency of the different approaches.

[1] S Chelkowski, A D Bandrauk & P B Corkum, "Efficient Molecular Dissociation by a Chirped Ultrashort Infrared Laser Pulse", *Physical Review Letters*, 65(19), 2355–8 (1990).

[2] J M Sanz-Serna & A Portillo, "Classical numerical integrators for wave-packet dynamics", *J. Chem. Phys.*, 104(6), 2349–55 (1996).

PRESERVING QUALITATIVE BEHAVIOUR AND TRANSIENCE IN NUMERICAL SOLUTIONS OF VOLTERRA INTEGRO-DIFFERENTIAL EQUATIONS OF CONVOLUTION TYPE: LYAPUNOV FUNCTIONAL APPROACHES

J A Roberts & N J Ford (*University College Chester, Department of Mathematics, Chester CH1 4BJ, UK*)

In this work we consider equations of the form

$$y'(t) = - \int_0^t k(t-s)g(y(s))ds, \quad t \in \mathbb{R}^+,$$

and the corresponding discretised equation of the form

$$y_{n+1} - y_n = -h^2 \sum_{j=0}^{n+1} w_j^{(n+1)} A_{n+1-j} g(y_j), n \in N.$$

We use a discrete Lyapunov function to analyse the stability of the continuous problem, basing our analysis on material given by Levin and Nohel in their discussion. We give

a theorem on the qualitative behaviour of solutions to the discrete problem and we are able to extend the analysis of both the continuous and discrete equations to a wider class of equations. We consider what conditions should be imposed on the numerical method to guarantee that the qualitative behaviour of solutions of the continuous problem will be preserved in the solutions of the discrete equations.

EXTRAPOLATION TECHNIQUES FOR ILL-CONDITIONED LINEAR SYSTEMS

G Rodriguez (*Universita' di Cagliari, Dipartimento di Matematica, viale Merello 92, 09123 Cagliari, Italy*)

In this talk, the regularized solutions of an ill-conditioned system of linear equations are computed for several values of the regularization parameter λ . Then, these solutions are extrapolated at $\lambda = 0$ by various vector rational extrapolations techniques built for that purpose. These techniques are justified by an analysis of the regularized solutions based on the singular value decomposition and the generalized singular value decomposition. Numerical results illustrate the effectiveness of the procedures.

CALCULATION OF EVOLUTIONARY STABLE STRATEGIES FOR POPULATION MODELS WITH PERIODIC OR CHAOTIC ATTRACTORS

S W Schoombie (*University of the Orange Free State, Dept. of Mathematics and Applied Mathematics, PO Box 339, Bloemfontein 9300, South Africa*)

Discrete versions of certain biological growth models have become models in their own right. The solutions of some of these show periodic or chaotic behaviour, depending on the values of certain parameters. It is of interest to biologists to find the optimal values of such parameters, in the sense that a species with some property or properties described by such an optimal parameter value, can not be invaded by a mutant species with a different value of the parameter. In such a case the parameter is called a Evolutionary Stable Strategy (ESS). An ESS corresponds to a maximum value of a certain Lyapunov exponent. Here we show that a simple difference scheme proposed by Vincent and Brown, would lead to such an optimal value, even in the case of periodic or chaotic models. We illustrate this, using a population model which has only periodic or chaotic ESS's.

ON COMPUTING EIGENVALUES OF THE DISCRETIZED NAVIER STOKES EQUATION

J Scott & R B Lehoucq (*Rutherford Appleton Laboratory, Didcot, OXON OX11 0QX, UK*)

In this talk we are concerned with finding the leftmost eigenvalues of large sparse nonsymmetric generalized eigenvalue problems which arise in stability studies of incompressible fluid flow. The matrices have a block structure that is typical of mixed finite element discretizations for such problems. We compare the use of shift-invert and Cayley transformations in conjunction with subspace iteration and the implicitly restarted Arnoldi method. Numerical results are presented for some model problems arising from the EN-TWIFE finite element package.

IMPLEMENTATION OF HOPF AND DOUBLE HOPF ALGORITHMS IN CONTENT

B Sijnave, W Govaerts & Y Kuznetsov (*Universiteit-Gent, B9000 Gent, Belgium*)

A Hopf point of a dynamical system is an equilibrium solution where the Jacobian matrix has a conjugate pair of complex eigenvalues with real part zero. It is a double Hopf point

if there are two such pairs. These cases have important dynamical implications and can be computed using bordered matrices.

In this talk, we discuss the computational study of curves of Hopf and double Hopf points in the software package CONTENT developed at CWI, Amsterdam by Y. A. Kuznetsov and V. V. Levitin. The bialternate product of matrices is extensively used in two codes for single Hopf and one for double Hopf. In the double Hopf and one of the single Hopf cases this is combined with a bordered matrix method.

We illustrate the use of this software with model computations, including the computation of a double Hopf curve in a realistic model of a neuron, developed at Cornell university by J. Guckenheimer and co-workers. The appearance of double Hopf points in such models is a noteworthy phenomenon.

HIGHLY-ACCURATE FAR-FIELD CONDITIONS FOR STATIONARY 3D TRANSONIC AERODYNAMIC PROBLEMS

I Sofronov & W L Wendland (*Keldysh Institut of Applied Mathematics RAS, Moscow, Russia*)

We consider the problem of constructing non-reflecting and highly-accurate far-field conditions for 3D transonic aerodynamics. The far field is supposed to be described by Euler equations linearized about uniform flow at infinity (such model has a good potential because of vanishing viscous and nonlinear effects far from the stream-lined body).

Our far-field conditions are exact with respect to linearized Euler equations. In order to obtain them, we decompose the governing equations for perturbations (u, v, w, P, ρ) of (x, y, z) components of velocity $\mathbf{V}_\infty + \mathbf{V}$, pressure $P_\infty + P$, and density $\rho_\infty + \rho$ into two transport equations for u and ρ and the subsystem

$$\text{rot} \mathbf{E} = \mathbf{b}, \quad \text{div} \mathbf{E} = 0$$

for the vector $\mathbf{E} = (-P, v, w)$ where the function $\mathbf{b}$ vanishes outside a wake domain and depends on (y, z) in the wake. By using Green's formula, we write out the representation formulae of general solution to our system outside the computational domain. The representation operator has a special projector-type form and consists only of surface integrals, i.e., it maps arbitrary data (u, v, w, P, ρ) given on the surface of the computational domain into the set of solutions of the linearized Euler equations.

This operator is used then to construct a numerical procedure of imposing far-field conditions for transonic flow problems. In order to provide the required accuracy of the numerical integration, we apply the exact analytical formulae of convolving integral kernels with bilinear functions given on a triangular surface.

THE MODELLING OF CHEMICALS LEAKAGE FROM THE WASTE POND

M Stýblo, J Maryška, J Novák, P Mareček & J Mužák (*Czech Technical University, Department of Mathematics, FNSPE CTU Prague, Trojanova 12, 120 00 Prague 2, Czech Republic*)

The application of finite-volume scheme on modelling of waste leakage is considered. The paper contains a short description of the hydrogeological condition, the overview of computational method and a presentation of computed results.

OPTIMAL APPROXIMABILITY OF SOLUTIONS OF SINGULARLY PERTURBED LINEAR REACTION-DIFFUSION PROBLEMS IN TWO DIMENSIONS

M Stynes & R B Kellogg (*University College Cork, Department of Mathematics, Ireland*)

We consider a linear singularly perturbed reaction-diffusion problem in a two-dimensional domain. While many numerical methods have been applied to solve such problems, no theory exists that analyses the optimality (or otherwise) of these methods in terms of the smoothness of the solution of the problem and of the value of the singular perturbation parameter; small values of this parameter often cause a significant deterioration in the accuracy of a computed solution. Using the theory of n -widths, we give results that clarify the best possible rates of convergence that can be attained in the L_2 norm.

BOUNDARY ELEMENT METHOD SOLUTION OF ELECTRICALLY DRIVEN MAGNETOHYDRODYNAMIC FLOW IN A RECTANGULAR DUCT

M Tezer-Sezgin (*Middle East Technical University, 06531 Ankara, Turkey*)

The magnetohydrodynamic (MHD) flow of an incompressible, viscous, electrically conducting fluid in a rectangular duct with an external magnetic field applied transverse to the flow has been investigated. An electric current travels between the electrodes, placed parallel to each other in the middle of the non-conducting walls, which are perpendicular to the applied magnetic field. The flow is driven by the current produced by these electrodes. The other two walls are non-conducting.

The boundary element method (BEM) with constant elements has been used to cast the problem into the form of an integral equation over the boundary and to obtain a system of algebraic equations for the boundary unknown values only.

The solution of this integral equation presents no problem as encountered in the solution of the singular integral equations for interior methods. Computations have been carried out for several values of the Hartmann number ($1 \leq M \leq 10$). It is found that as M increases, boundary layers are formed close to the non-conducting walls for the velocity field. Induced magnetic field lines (current lines) are perpendicular to the electrodes demonstrating the normal derivative condition as zero. Several graphs are given showing the behaviours of the velocity and the induced magnetic field.

SHOOTING AND GLOBAL TECHNIQUES FOR DIFFERENTIAL-ALGEBRAIC BOUNDARY VALUE PROBLEMS ARISING IN DETONATION MODELLING

R M Thomas (*UMIST, Department of Mathematics, Manchester, UK*)

The modelling of detonation often gives rise to a parameterised free boundary value problem containing differential and algebraic equations, modelling chemical kinetics, fluid flow and conservation laws. The physics can be modelled simply or in more complicated fashions and, depending upon the detonation velocity, solutions may or may not exist.

We investigate a model of unconfined detonation. The mathematical model can be formulated as either a fully-implicit DAE or as a semi-explicit DAE or as an ODE. We discuss the advantages and disadvantages of shooting and global techniques for the various formulations and we present some numerical results.

OPTIMISING THE MESH IN THE DISCRETISATION OF HYPERBOLIC PROBLEMS

Y Tourigny (*University of Bristol, School of Mathematics, UK*)

One of the main objections commonly raised against mesh optimisation is that the added computational complexity far outweighs the gain in accuracy. Recently however, Tourigny and Hülsemann developed a new approach, applicable to finite element discretisations of variational problems, in which the mesh is optimised by solving a sequence of *local* partial differential problems. With this approach, the cost of optimising the mesh is comparable to that of solving the *global* discrete problem on a given mesh. In this talk, which naturally follows from that of Hülsemann, I will explain how such ideas may also be used in the context of hyperbolic problems.

SYMBOLIC BOUNDARY APPROXIMATION METHODS FOR MOTZ PROBLEM

Tzon-Tzer Lu & Ming-Yuh Horng (*National Sun Yat-sen University, Taiwan, Department of Applied Mathematics, Kaohsiung, Taiwan*)

We use boundary approximation method to solve Motz problem, an elliptic boundary value problem with singularity. Piecewise particular solutions in subdomains are employed to approximate boundary and interface conditions as best as possible. We combine numerical and symbolic techniques to get the most accurate solution ever published. We also solve Motz problem under different divisions of the domain and get very accurate solutions. All methods are fully analyzed and compared.

ON THE CONSTRUCTION OF P-STABLE MIRKN-OUT OF MIRK-METHODS

G Vanden Berghe, H De Meyer, T Van Hecke & M Van Daele (*University of Gent, Vakgroep Toegepaste Wiskunde en Informatica, B9000 Gent, Belgium*)

For the numerical solution of second order IVP of the type $y'' = f(x, y)$, $y(0) = a$, $y'(0) = b$, we consider the particular class of Runge-Kutta Nyström methods (RKN) obtained by the application of mono-implicit Runge-Kutta methods (MIRK) on the equivalent first order IVP $y' = z$, $z' = f(x, y)$, $y(0) = a$, $z(0) = b$.

We investigate the conditions under which an implicit *RKN* method that is generated by a MIRK method, is itself mono-implicit (MIRKN) and P-stable and we show that these conditions can be formulated as simple constraints on the MIRK method.

Making use of the general classification of s -stage MIRK methods ($s \leq 5$), recently established by Burrage et al., and of the so-called multistride MIRK methods which were investigated by the present authors, examples of P-stable MIRKN methods of various order and various stage order are given.

ON A CLASS OF MONO-IMPLICIT RUNGE-KUTTA-NYSTROM METHODS

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Among the implicit Runge-Kutta-Nyström methods (IRKN) determined by the Butcher tableau

$$\begin{array}{c|c} c & A \\ \hline & \bar{b} \\ & b \end{array}$$

with $c, \bar{b}, b \in \mathbb{R}^{s \times 1}$ and $A \in \mathbb{R}^{s \times s}$, we consider the subclass of mono-implicit methods (MIRKN), and more in particular the MIRKN methods for which a strictly lower triangular matrix $X \in \mathbb{R}^{s \times s}$ and a vector $v \in \mathbb{R}^{s \times 1}$ exist such that the Butcher matrix A can

be written as

$$A = X + v\bar{b}^T.$$

Moreover, since we aim at the construction of P-stable MIRKN methods, we require that the 2×2 matrix stability function

$$M(z) = \begin{bmatrix} 1 + z\bar{b}^T(I - zA)^{-1}e & 1 + z\bar{b}^T(I - zA)^{-1}c \\ zb^T(I - zA)^{-1}e & 1 + zb^T(I - zA)^{-1}c \end{bmatrix},$$

whereby $e \in \mathbb{R}^{s \times 1}$ denotes the vector with unit entries, satisfies for all real $z < 0$ both the conditions $\det M(z) = 1$ and $(\text{Tr} M(z))^2 < 4$.

We show that for any s -stage MIRKN method of order at least s , the first condition is satisfied if one chooses $v = c$ and $X^{\lfloor s/2 \rfloor} = 0$. Further exploration of the subclass of MIRKN methods corresponding with this particular choice of v and X , reveals a standard procedure for the construction of P-stable MIRKN methods with an even number of stages s , having order s and stage order $q = \min\{s, 4\}$. Several examples are given to illustrate this procedure.

STABILITY RESULTS ON SOME DIRECT QUADRATURE METHODS FOR VOLTERRA INTEGRO-DIFFERENTIAL EQUATIONS

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The numerical stability of the Direct Quadrature methods based on Backward Euler and Trapezoidal formulas for linear systems of Volterra integro-differential equations with convolution kernel is analyzed.

We perform a parallel analysis for the stability of the continuous and discrete problem and in particular we prove some conditions assuring that the numerical solution furnished by the above methods presents stability properties analogous to the ones of the analytical solution.

Moreover some conditions on the characteristics of the considered integro-differential equation and on the discretization step are given in order to obtain that the global error of the Backward Euler methods decays. Such conditions can be considered as a generalization to the vectorial case of the known results on the stability of the methods applied to the scalar test integro-differential equation.

SPURIOUS FIXED POINTS OF AN ADAPTIVE PREDICTOR CORRECTOR ALGORITHM

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It is commonly accepted that fixed step size predictor corrector algorithms for the numerical solution of initial value problems permit spurious fixed points. We consider how this concept extends to one particular adaptive (variable step size, variable order) predictor corrector algorithm of Shampine and Gordon. We show that the algorithm can permit spurious fixed points and construct an example of this behaviour. However, we also show that any spurious fixed point will have a residual that is of the order of the error tolerance. Further, we argue that spurious fixed points are unlikely to occur in practice.

DISCRETE PROJECTIONS ONTO WAVELET SUBSPACES

A F Ware (*University of Durham, Department of Mathematical Sciences, UK*)

Given a bounded continuous function f , there exist linear functionals, each involving a finite number of samples of f , that act as projections onto spaces spanned by Daubechies scaling functions and wavelets. The coefficients of f calculated using these discrete projections are related to the true values by an analogue of the Poisson summation formula relating the discrete Fourier transform to the continuous Fourier transform. The error from such a projection carried out at one resolution level can then be expanded entirely in terms of wavelet coefficients of f at higher resolution levels. The resulting possibility of adaptive wavelet-based quadrature is investigated.

A HIGH PERFORMANCE LINEAR ALGEBRA PACKAGE, LAPACK IN FORTRAN 90

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The purpose of this paper is to discuss the design of a Fortran 90 interface to LAPACK. Our emphasis at this stage is on the design of an improved user-interface to the package, taking advantage of the considerable simplifications which Fortran 90 allows. The proposed design makes use of assumed-shape arrays, optional arguments, and generic interfaces. All the LAPACK driver and some computational routines are already implemented for FORTRAN'90.

SOME MATRIX APPROXIMATION PROBLEMS IN CONTROL THEORY

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Algorithms based on simple iteration combined with a checking step are developed for two problems in control theory: computing the distance to instability of a stable matrix and computing the H_∞ norm of a transfer matrix. The checking step corresponds to one used in the bisection method, which is currently a popular approach to solving these problems. The new approach has potential efficiency gains.

ADAPTIVE WAVELET ADI METHODS FOR TWO DIMENSIONAL FLAME PROPAGATION

Wei Cai (*University of North Carolina at Charlotte, Department of Mathematics, Charlotte, NC 28223, USA*)

In this talk, we will extend our one dimensional wavelet collocation methods for initial boundary value problems of PDEs (SIAM J. NA, June 1996) to the case of two dimensional problems with an ADI factorization for efficient time marching. The spline wavelet is constructed for the Sobolev space $H^2(I)$ on a closed interval with additional boundary wavelets and scaling functions. The wavelet basis from these special wavelet functions forms a hierarchical basis over the proposed collocation points. As a result, a fast discrete wavelet interpolation transform between function values and wavelet interpolation expansion coefficients is achieved with $O(n \log n)$ complexity. The two dimensional wavelet scheme coupled with ADI methods provides the advantage of both local mesh refinement of finite element methods and efficient solver property of the traditional ADI methods. Numerical results for two dimensional flame propagations will be presented.

NUMERICAL INSIGHTS INTO THE BEHAVIOUR OF APPROXIMATE SOLUTIONS TO DELAY

DIFFERENTIAL EQUATIONS NEAR TO A HOPF BIFURCATION POINT

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We are interested in the preservation of properties in the solution of delay differential equations by numerical methods. Previous work gives good insight into the approximation of solutions near asymptotically stable equilibrium points. In our work we concentrate on the behaviour close to a Hopf bifurcation.

In this talk, we present initial insights related to a simple class of methods applied to a well-known delay equation:

We consider the θ -method applied to the delay logistic equation $\dot{x}(t) = -\lambda x(t-1)[1+x(t)]$. It is known that the analytic solution undergoes a Hopf bifurcation at $\lambda = \pi/2$. Our numerical experiments suggest that the θ -method generates a dynamical system with an attracting periodic orbit if the parameter λ is near $\pi/2$.

We discuss how this corresponds to the behaviour of the method applied to ODEs with periodic solutions. We give some insight that indicates under which conditions the method will preserve the qualitative behaviour of the delay logistic equation near the Hopf bifurcation.

WAVEFORM RELAXATION METHOD FOR NONLINEAR DIFFERENTIAL-FUNCTIONAL EQUATIONS

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In this talk, we will consider the waveform relaxation method for solving a general class of nonlinear functional differential equations. This class includes ordinary differential equations, delay equations, as well as integro-differential equations. The system of differential equations could be derived from application of the method of lines approximation of a partial functional-differential equation. New error estimations under linear and nonlinear conditions for the right hand side of the system of equations will be presented. A benefit of the application of the nonlinear condition will be shown. Numerical experiments will also be presented. Actual and theoretical errors will be compared.