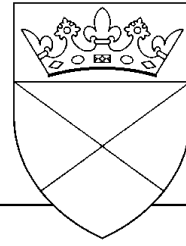


University
Of Dundee



MATHEMATICS & COMPUTER SCIENCE

16th Biennial Conference
on
Numerical Analysis

27 June—30 June, 1995

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Compiled by David F. Griffiths and Desmond J. Higham.

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 Airlie 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 Airlie 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 Bonar Hall from 20.00 to 22.00 on Tuesday 28 June.

8. Conference Dinner

The conference dinner will be held in Bonar Hall on Thursday 29 June at 20.00, and sherry will be provided beforehand from 19.30. The guest speaker will be Professor John Butcher, University of Auckland.

Abstracts of Invited Talks

INNER/OUTER ITERATIONS FOR SOLVING LINEAR SYSTEMS OF EQUATIONS

Gene H. Golub (Stanford University, U.S.A.)

We consider solving the linear system of equations $Ax = b$. In many situations, it is natural to rewrite the system as $Mx = Nx + b$. This leads to the iteration

$$Mx^{k+1} = Nx^k + b. \quad (1)$$

We can replace the equation (1) by the equivalent system

$$Mz^k = r^k, \quad x^{k+1} = x^k + z^k, \quad (2)$$

where $r^k = b - Ax^k$. We have assumed that it is ‘easy’ to solve the system (2). Unfortunately, we may have to perform inner iterations to solve (2) so that we replace the algorithm described by (2) by

$$M\bar{z}^k = r^k + q^k, \quad x^{k+1} = x^k + \bar{z}^k. \quad (3)$$

The vector q^k is the residual vector associated with the inner iteration; we continue to iterate until $\|q^k\| \leq \tau_k \|r^k\|$. The parameters $\{\tau_k\}$ play an important role in the convergence analysis, and we describe various strategies for choosing $\{\tau_k\}$. Our analysis will be independent of the method used for solving the system (3) and the inner iteration.

There are numerous problems that fit into the framework we have described. In particular, inner and outer iterations play an important role in domain decomposition, solution of non-symmetric systems where the coefficient matrix is real, positive and in the implementation of the method of Uzawa in solving the Stokes equation. Furthermore, we can apply these ideas to using Chebyshev polynomials for the acceleration of various iterative methods where fast direct methods are used for the inner iteration. We describe the results of various numerical experiments.

ODE SOLVING WITH AUTOMATIC DIFFERENTIATION AND RATIONAL PREDICTION

Andreas Griewank (Technical University Dresden, Germany)

For any autonomous right hand side defined by an evaluation procedure written in C (or Fortran90), one can compute time-derivatives of the state up to any order by automatic differentiation. This chain-rule based technique can also be used to calculate the time-derivatives of the Jacobian along the solution paths at a reasonable expense. As it turns out these square matrices also represent the Jacobians of the state-vector-derivatives with respect to the current state vector itself. If the right hand side is non-smooth due to the appearance of absolute values or general branches in its evaluation procedure, then one can still obtain one-sided derivatives and identify test functions whose roots with respect to time determine the discontinuities. All this information is obtained with working accuracy at a price that grows at worst quadratically with the number of time derivatives required.

Using the time-derivatives of the state and their Jacobians one can implement the Hermite interpolation based Obrechkov methods named and analyzed by Wanner in a straight forward manner. On linear systems these one step methods are equivalent to implicit Runge-Kutta methods and therefore have the same desirable A- and L-stability properties. On dense nonlinear systems the linear algebra effort per step is somewhat lower

but the evaluation effort is slightly larger than the corresponding costs for IRK methods. Irrespective of such asymptotic comparisons, it is crucial that sparsity in the right hand side be exploited and that large steps are facilitated through good state prediction and error estimation techniques.

For stiff systems we report encouraging results with a predictor based on polynomial approximations to the Jacobian along the solution path. Further improvements are expected through the use of Pade approximants in the noncommutative algebra of square matrices. In either case the resulting state predictor is a rational function of the derivative data and its order is more than half that of the underlying Obrechkov method so that one Newton correction usually suffices. Finally, the available derivative information provides several ways to estimate the discretization error and to select the next step-size and order.

The talk will describe the derivative information available, report their use in our experimental Obrechkov code for stiff and highly oscillatory problems, and discuss possible extensions to other problem classes like DAEs.

DISCRETISED EIGENVALUE PROBLEMS, LBB CONSTANTS AND STABILIZATION

D. F. Griffiths (University of Dundee)

Certain discretised eigenvalue problems give rise to eigenvalues that converge as the grid size is reduced yet are spurious in the sense that the corresponding eigenvectors are nonphysical. We shall discuss this problem in the context of the Babuska–Brezzi condition and describe possible means of stabilizing the discretizations.

MULTIDIMENSIONAL SCHEMES FOR NONLINEAR SYSTEMS OF HYPERBOLIC CONSERVATION LAWS

Rolf Jeltsch (Federal Institute of Technology, Switzerland) *Michael Fey* (California Institute of Technology, U.S.A.) & *A.-T. Morel* (Federal Institute of Technology, Switzerland).

Most commonly used schemes for unsteady multidimensional systems of hyperbolic conservation laws use dimensional splitting. In each coordinate direction a scheme for a one dimensional system is used. Such an approach does not take in account the infinitely many propagation directions which are present in a system in several space dimensions. In 1992 M. Fey introduced what he called the **M**ethod of **T**ransport, MoT, for the Euler equations of gas dynamics. It is a finite volume method which uses the transport along characteristics. It does not compute fluxes across cell sides but from one cell to another. Fey and Morel have shown that this scheme can also be used for the magnetohydrodynamic equations and the shallow water equation. Ostkamp has recently proved convergence of the MoT when applied to the linear, constant coefficient wave equation. She also interpreted the MoT as an Euler Characteristic Galerkin method. While the original MoT is first order only Fey and Morel give second order extensions of the scheme. In this lecture an overview of recent developments is given.

VARIATIONAL ERROR BOUNDS FOR RADIAL BASIS FUNCTIONS

Will Light (University of Leicester)

Suppose $x_1, \dots, x_m$ are points in $\mathbb{R}^n$ at which real data $d_1, \dots, d_m$ are given. If the points are very scattered, or the dimension n is very high, then piecewise polynomials are difficult to use because the process of constructing a suitable triangulation is hard. For such problems, interpolation by radial basis functions is felt to be a good technique.

(That was a deliberately cautious sentence. There remain problems with the numerical implementation of radial basis methods!) The interpolation subspace is constructed by first choosing a function $\phi : \mathbb{R} \rightarrow \mathbb{R}$ and a natural number k . The subspace then consists of all functions s of the form

$$s(x) = \sum_{i=1}^m a_i \phi(|x - x_i|) + p(x), \quad x \in \mathbb{R}^n,$$

where p is a polynomial of degree at most k , and $a_1, \dots, a_m$ are real numbers satisfying

$$\sum_{i=1}^m a_i q(x_i) = 0 \quad \text{for all } q \text{ which are polynomials of degree at most } k.$$

The interpolation problem is then to determine whether a unique choice of $a_1, \dots, a_m$ and p exists so that $s(x_j) = d_j$ for $j = 1, \dots, m$.

The immediate question about such a setup is whether interpolation is possible independent of the location of the knots $x_1, \dots, x_m$. If things are done properly, the interpolant can be viewed as minimising a certain seminorm. We will show

1. the fundamental error bounds of Golomb and Weinberger (familiar stuff to many of you!).
2. the variational treatment of Duchon, which is very close to parts of the finite element theory.
3. the variational treatment of Madych and Nelson, which comes from the theory of conditionally positive definite functions.
4. how to obtain improved error bounds over the Golomb-Weinberger theory.

FINITE VOLUME METHODS

K.W. Morton (University of Oxford)

To a numerical analyst, finite volume methods are low order, non-conforming Petrov-Galerkin methods of no particular significance. But to the aeronautical engineer they are key design tools, well suited to the efficient modelling of nonlinear conservation laws in complicated three-dimensional geometries. In view of their dominance in this area of computational fluid dynamics, and because of the need to resolve a number of important issues and make improvements in key areas, these methods merit and require more attention from numerical analysts.

In this lecture, I will briefly review the range of methods on structured and unstructured meshes that are in use, and their links to more familiar finite difference and finite element methods. This will be followed by a selection from the numerical analysis results that have been established, particularly in regard to their robustness for singular perturbation problems. Finally, I will outline some of the outstanding issues and situations for which more analysis is needed. In each case the cell vertex scheme will be used as a key exemplar of the methods.

ORTHOGONAL EIGENVECTORS WITHOUT GRAM-SCHMIDT

B. N. Parlett (University of California at Berkeley, U.S.A.)

The goal is to compute approximate eigenvectors for symmetric tridiagonal matrices that are orthogonal to working accuracy however close the eigenvalues may be to each other. Methods based on inverse iteration seem obliged to invoke the Gram-Schmidt orthogonalization process to achieve the goal and that is bad news for parallel processing. We present the theory behind a different approach. If there is a cluster of m eigenvalues in an interval $\mathcal{I}$ of width $|\mathcal{I}|$ that is separated by a reasonable gap g from the rest of the spectrum then one may choose m submatrices each of which overlaps only its nearest neighbours and has a simple eigenvalue θ_i in $\mathcal{I}$, $i = 1, \dots, m$. For a cluster of size 3 the submatrices might be 1 : 30, 15 : 50, 40 : 80. By padding θ_i 's eigenvector with 0's one obtains m normalized big vectors $\mathbf{p}_1, \dots, \mathbf{p}_m$ with $\mathbf{p}_i \bullet \mathbf{p}_j = 0$, if $|i - j| > 1$. The residual norm of each $\mathbf{p}_i$ is $O(|\mathcal{I}|)$ and, for the vectors of absolute values $|\mathbf{p}_i|$ we show that $|\mathbf{p}_i| \bullet |\mathbf{p}_{i+1}| = O((|\mathcal{I}|/g)^{3/4})$. When necessary one can replace each $\mathbf{p}_i$ by $\mathbf{q}_i = \mathbf{p}_i - \mathbf{p}_{i-1}(\mathbf{p}_{i-1} \bullet \mathbf{p}_i) - \mathbf{p}_{i+1}(\mathbf{p}_{i+1} \bullet \mathbf{p}_i)$. In most cases $\mathbf{p}_i \bullet \mathbf{p}_{i+1}$ may be inferred from known quantities and then no dot products are needed at all.

We will show pictures of some examples.

TO BE ANNOUNCED

Linda Petzold (University of Minnesota, U.S.A.)

MOVING MESH METHODS, WITH APPLICATIONS TO BLOW-UP PROBLEMS FOR PDES

Robert D. Russell (Simon Fraser University, Canada)

Of the two basic adaptive approaches for solving time dependent partial differential equations, the dynamic approach has proven to be considerably less popular than the static one. In this talk we shall discuss a dynamic (or moving mesh) approach which is based upon the use of so-called moving mesh PDEs (MMPDEs). Various theoretical results about this approach and a description of the basic mesh smoothing strategy are given. Then a finite difference approach and an alternative moving mesh collocation method are introduced. The collocation method, based upon solving PDEs in divergence form (at this point, in one space dimension) uses a cell-averaging type cubic Hermite collocation discretization for the physical PDEs and a three point finite difference discretization for the MMPDE which determines the moving mesh. The methods are applied to problems displaying a variety of different solution behaviours. Special emphasis is given to problems in combustion theory, where scaling invariance of the solutions leads to intriguing new applications of the methods.

EFFICIENT PRE AND POSTPROCESSING OF SYMPLECTIC INTEGRATIONS

J. M. Sanz-Serna (Universidad de Valladolid, Spain) *M. A. Lopez-Marcos* (Universidad de Valladolid, Spain) & *R. D. Skeel* (University of Illinois at Urbana-Champaign, U.S.A.).

We show how to increase the accuracy of symplectic integrations by cheaply processing the results given by the numerical method being used. The numerical results will focus on an application to molecular dynamics.

FAST & ROBUST SOLVERS FOR TIME-DISCRETISED INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

David Silvester (UMIST) & *Andrew Wathen* (University of Bristol).

In this talk we consider the design of robust and efficient methods for solving the Navier-Stokes equations governing laminar flow of a viscous incompressible fluid.

Three fundamental issues will be assessed in detail: the discretisation of the convective transport terms, the (weak-) enforcement of the incompressibility constraint in a mixed finite element setting, and the solution of the indefinite (Stokes-) systems arising at each time-level. Our aim is to prescribe a framework for adaptive error control. The essential ingredients are: an unconditionally stable time-discretisation; “natural” spatial discretisations which are (inf-sup) stable; and a fast iterative solution strategy generating iterates converging monotonically in an appropriate norm (which mimics the dissipation inherent in the continuous system).

A distinguishing feature of our methodology is the use of multigrid preconditioning to accelerate the convergence of our Krylov subspace iterative solver. We motivate this with some analysis showing that the contraction rate is bounded away from unity independently of the choice of the mixed finite element method and the subdivision parameter. Analysis and implementation of “pure” multigrid methods seems to be relatively complicated and (discretisation-) method dependent by comparison.

For background information, see [1] and [2].

[1] A. Wathen & D. Silvester, Fast iterative solution of stabilised Stokes systems part I: using simple diagonal preconditioners, SIAM Journal of Numerical Analysis, v.30, pp. 630–649 (1993).

[2] D. Silvester & A. Wathen, Fast iterative solution of stabilised Stokes systems part II: using general block preconditioners, SIAM Journal of Numerical Analysis, v.31, pp. 1352–1367 (1994).

A POSTERIORI ERROR ANALYSIS AND GLOBAL ERROR CONTROL FOR ADAPTIVE FINITE VOLUME APPROXIMATIONS OF HYPERBOLIC PROBLEMS

Endre Süli (University of Oxford)

Due to their inherent local conservation properties and ease of application on irregular multi-dimensional domains, finite volume methods have become one of the most popular numerical techniques for the approximate solution of partial differential equations of compressible gas dynamics.

In this talk we describe a theoretical framework for the *a posteriori* error analysis of finite volume methods. Initially we consider linear hyperbolic systems and exploit an error-localisation procedure: the global error is decomposed into a locally generated part $\mathbf{e}_{loc}$ which is directly controlled by the computable residual $\mathbf{r}$, and a propagating component $\mathbf{e}_{trans}$ which represents the accumulation of errors generated upwind of an element and merely transmitted through it. Thus we obtain two-sided local error bounds of the form

$$c_0 \|\mathbf{r}\|_{H'(L,K)} \leq \|\mathbf{e}_{loc}\|_{L^2(K)} \leq c_1 \|\mathbf{r}\|_{H'(L,K)},$$

where $\|\cdot\|_{H'(L,K)}$ is the dual graph-norm associated with the hyperbolic operator L on the element K , and c_0 and c_1 are computable constants. By using a local Gårding inequality, we further prove that

$$c_2 \|h_0 P_{h_0} \mathbf{r}\|_{L^2(K)} \leq \|\mathbf{e}_{loc}\|_{L^2(K)} \leq c_3 \|h \mathbf{r}\|_{L^2(K)},$$

where, again, c_2 and c_3 are computable constants, h denotes the diameter of K , h_0 is a mesh-size of a micro-partition of K , and P_{h_0} is the orthogonal-projector onto a finite element subspace $S_{h_0}(K) \subset L_2(K)$ defined on this micro-partition. We describe how these *a posteriori* error bounds may be used in designing local error indicators and global error estimators, and discuss the extension of the theory to nonlinear systems of conservation laws.

The theoretical results are illustrated by numerical experiments which highlight the potential of this approach in the design of adaptive finite volume approximations of linear and nonlinear hyperbolic problems.

DIRECT SEARCH METHODS: ONCE SCORNE, NOW RESPECTABLE

Margaret H. Wright (AT&T Bell Laboratories, USA)

The need to optimize a function whose derivatives are unknown or non-existent arises in many contexts, particularly in real-world applications. Various direct search methods, most notably the Nelder-Mead ‘simplex’ method, were proposed in the early 1960s for such problems, and have been enormously popular with practitioners ever since. Nonetheless, for 25 years these methods were typically dismissed or ignored in the mainstream optimization literature, primarily because of the lack of rigorous convergence results. Since 1989, however, inspired by parallel computing, direct search methods have been rejuvenated and made respectable. This talk will survey direct search methods, describe recent developments, and discuss potential future theoretical directions and practical applications.

HOW CAN NONSMOOTH METHODS HELP IN OPTIMIZATION OF MECHANICAL STRUCTURES?

Jochem Zowe (University of Bayreuth, Germany)

We discuss the modelling of discrete mechanical structures consisting of n nodes and m nodal connections (so-called trusses like bridges, electricity masts etc.). The aim is to choose the design variables (bar sizes and nodal positions) such that the structure becomes as stiff as possible with respect to a given load. The mechanical-mathematical modelling leads to a nonconvex constrained optimization problem in $n + m$ design and m state variables.

Already for planar models, n and m will be of the order of 10^2 – 10^3 and 10^3 – 10^5 , respectively; thus classical software has no chance in this context. We discuss how nonsmooth optimization helps to overcome these difficulties. Examples will demonstrate the efficiency of this concept.

Abstracts of Submitted Talks

THE RATE OF CONVERGENCE OF THE p -VERSION FINITE ELEMENT METHOD FOR NON-LINEAR ELLIPTIC PDES.

Mark Ainsworth (University of Leicester) & *David Kay* (University of Leicester).

Traditionally it was thought that there was little point in using high order finite elements to approximate solutions of PDEs since the rate of convergence is limited by the smoothness of the solution. However, for linear elliptic problems it has been shown that the p -version finite element method (in which the polynomial degree is increased) converges at twice the rate of the classical h -version.

The current work deals with the rate of convergence of the p -version for *non-linear* elliptic problems. New approximation theoretic results are obtained for approximation using piecewise polynomials of degree p on meshes of triangular and quadrilateral elements. Estimates for the rate of convergence in Sobolev spaces $W^{m,q}(\Omega)$, $q \in [1, \infty]$ are given. These are then used to obtain the rate of convergence when the p -version is used to solve the α -Laplacian. Numerical examples are given illustrating the theory.

ON THE INITIAL HESSIAN APPROXIMATION FOR THE LIMITED MEMORY BFGS METHOD FOR LARGE SCALE OPTIMIZATION

M. Al-Baali (UAAE University, United Arab Emirates)

In the limited memory BFGS (L-BFGS) method for large scale optimization, the Hessian approximation is defined as the outcome of updating a given matrix, say D , by using the BFGS formula and certain other information. A useful choice for D is defined by the unit matrix multiplied by a certain scalar (Nocedal and Liu, 1989, Math. Prog. Vol 45). In this talk we describe new nondiagonal choices for D without increasing the storage locations required by the L-BFGS method. We study numerical results, and show that our choices for D yield improvement over the best L-BFGS method of Nocedal and Liu.

STOPPING CRITERIA FOR ITERATIVE METHODS

Mario Arioli (Istituto di Analisi Numerica del C.N.R., Italy) *Eric Noulard* (Laboratoire d'Informatique et de Mathématiques Appliquées de l'E.N.S.E.E.I.H.T, France) & *Alessandro Russo* (Istituto di Analisi Numerica del C.N.R., Italy).

We introduce stopping criteria for iterations coming from PDE's. We show that, when we measure the residual of the linear system in the dual of the space where the PDE solution lies, we have real evaluation of the functional error, whereas the measure of the same residual with an algebraic norm can give misleading information about the convergence.

QUADRATURE AND DYNAMICS OF AN INTEGRO-DIFFERENTIAL EQUATION

M. A. Aves (University of Dundee) & *P.J. Davies, D.J. Higham* (University of Dundee).

The long-time dynamics of a discretised integro-differential equation are examined for two exponential integral kernels. Such an equation arises from a model of population growth where the growth rate is influenced by the size of previous populations. The stability of the fixed points and orbits of the numerical map is studied. Here emphasis is placed on the effect that quadrature has upon the asymptotic behaviour. Stable period-3 behaviour is shown to occur over a range of parameter values and a sufficient condition for the existence of period-3 solutions is presented. Finally a comparison of different quadrature formulae is made and how the issues raised pertain to their use in error-controlled Runge-Kutta methods.

AN ALGORITHM FOR GENERATING “BEST” UNSTRUCTURED MESHES IN A DISCRETE NORM BY SIMPLE AVERAGING

M.J.Baines (University of Reading)

In grid generation and adaptive PDE work there is a need for a simple algorithm for creating unstructured grids which are “best” in some sense. An algorithm is devised which, given an initial guess, moves the grid so as always reduce the error in a particular discrete norm. The steps of the algorithm are elementary and in particular the grid movement step bears a strong resemblance to an averaging procedure already employed in grid generation, thus providing a rationale for its use.

STABILITY ANALYSIS OF COLLOCATION RUNGE-KUTTA METHODS FOR VOLTERRA INTEGRO-DIFFERENTIAL SYSTEMS WITH UNBOUNDED DELAYS

Christopher T.H. Baker (The Victoria University of Manchester) & *Arsalang Tang* (The Victoria University of Manchester).

We have recently investigated conditions for the stability of solutions of variable-step collocation Runge-Kutta-based methods for linear and nonlinear delay Volterra differential equations (DVIDEs) with a “fading memory”. The methods are adaptations, using ideas from the treatment of Volterra integral equations, of corresponding collocation R-K methods for delay and ordinary differential equations. The basic tool of our stability analysis, and a novel feature of the paper, is the use of generalized Halanay inequalities. The analysis throws up some interesting questions related to Runge-Kutta methods for ODEs. The analysis is quite involved and we therefore sketch it in outline and dwell on some of its more accessible features. [The first-named author acknowledges support from EPSRC Mathematics Programme. The second-named author acknowledges support from The University of Manchester, the ORS scheme, and the Great Britain–China Educational Trust.]

JACOBIANS FOR ISOPARAMETRIC FINITE ELEMENTS

K. E. Barrett (Coventry University)

Isoparametric elements are only valid if the Jacobian determinant of the transformation between a given element and a master element does not change within or on the element boundary. Some algorithms are known which analyse Jacobians for various element types. Necessary conditions are presented for determining the validity of an element together with a novel geometrical interpretation. Detailed results are presented for deciding whether or not the Jacobian determinant for 6-noded and 8-noded elements change sign within an element given that the Jacobian is positive on the element edges. Some results are presented for a selection of three dimensional elements based on the two dimensional analysis.

APPLICATIONS OF MATHEMATICAL PROGRAMMING ALGORITHMS TO AGRICULTURAL PRODUCTION

John A. Belward (University of Queensland)Australia *David G. Mayer* (Animal Research Institute, Australia) & *Kevin Burrage* (University of Queensland, Australia).

Primary industries contribute a very significant proportion of Australia’s export income and a substantial share of that is contributed by Queensland’s Primary Producers. The Advanced Computing Group at the University of Queensland in cooperation with the Queensland Department of Primary Industries is applying High Performance Computing and Simulation and Modelling to the development of information packages, communica-

tions interfaces and decision support systems targeted at efficient sustainable agricultural production.

This presentation will describe a study of the performance of four sets of algorithms to a Multi-Dimensional Dairy Model.

A REGULARIZATION PROCEDURE FOR $\sum_{i=1}^n f_i(z_j)x_i = g(z_j), (j = 1, 2, \dots, n)$

G. Vanden Berghe (University of Gent, Belgium) & *H. De Meyer, M. Van Daele, L. Ixaru* (University of Gent, Belgium).

A regularization procedure for linear systems of the type $\sum_{i=1}^n f_i(z_j)x_i = g(z_j), j = 1, 2, \dots, n$ is presented, which is particularly useful in the case when $z_1, z_2, \dots, z_n$ are close to each other. Up to now, in all existing contributions, where such type of systems occur, one has avoided difficulties by just solving the system analytically. However, most of the time, finding the analytical solution of such a system is not a easy task. Even with the assistance of a computer algebra package the solution for n as large as five or six remains problematic. This kind of problems occurs in the derivation of the weights of the exponential-fitted multistep methods, used to solve second-order differential equations of the form $y'' = f(x, y)$. The derived numerical algorithm is tested on several examples in that field of interest for which analytical solutions do exist and is found to yield highly accurate results.

A MATRIX AND A FORMULA FOR THE BARYCENTRIC WEIGHTS OF RATIONAL INTERPOLATION

Jean-Paul Berrut (Université de Fribourg, Switzerland)

Let $x_0, \dots, x_N$ be $N + 1$ values of a real (or complex) variable x . Every rational interpolant r of a function f with numerator and denominator degrees $\leq N$ can be written in its barycentric form

$$r(x) = \frac{\sum_{k=0}^n \frac{b_k}{x - x_k} f(x_k)}{\sum_{k=0}^n \frac{b_k}{x - x_k}}$$

which is completely determined by the vector $\vec{b}$ of its $N + 1$ barycentric weights b_k . Finding $\vec{b}$ is therefore an alternative to the determination of the coefficients in the canonical form of r ; it is advantageous inasmuch as $\vec{b}$ contains information about unattainable points and poles. In classical rational interpolation the numerator and denominator of r are made unique (up to a constant factor) by restricting their respective degrees.

At least two methods for computing $\vec{b}$ are known: Schneider and Werner find the coefficients in the usual Newton form of the minimum degree denominator and in a second step transform them into $\vec{b}$. Another approach find $\vec{b}$ as the kernel of a Löwner matrix. In our talk we shall introduce another matrix whose kernel is the vector $\vec{b}$. Applying an elimination algorithm to this matrix then yields a formula for $\vec{b}$.

STABILITY OF KRYLOV SUBSPACE METHODS FOR LINEAR LEAST SQUARES PROBLEMS

Å. Björck (Linköping University, Sweden)

The conjugate gradient method applied to the normal equations $A^T A x = A^T b$ (CGLS) is a method of choice for solving large sparse linear least squares problems. The mathematically equivalent LSQR algorithm based on a Lanczos bidiagonalization process is an often recommended alternative. We investigate the achievable accuracy of such Krylov

subspace methods in finite precision. It is shown that implementations of CGLS, in which the residual $s_k = A^T(b - Ax_k)$ of the normal equations is recurred, cannot achieve accurate solutions. The same conclusion holds for the method based on Lanczos bidiagonalization with starting vector $A^T b$. Using recent results by Greenbaum and Strakos [1992] it is conjectured that for the preferred implementation of GGLS the normwise relative error in the recursive residual is of order machine precision. This result is supported by numerical tests. The achievable accuracy of LSQR is shown to be similar.

COLLOCATION FOR ABEL INTEGRAL EQUATIONS AND ITS STABILITY BEHAVIOUR

Luise Blank (Chester College)

For Abel integral equations of the second kind we investigate the the collocation approximation with polynomial splines. While the convergence of the method is well analyzed, the stability behaviour, i.e. the response of the solution to “admissible” perturbations, is still a fairly open field. For the case of the linear integral equation we characterize the stability domain in terms of the eigenvalues of the power series, which arises from the employed method. To exploit this characterization we provide a rigorous discussion of the boundary of the stability region. Finally, numerical illustrations of stability domains are given for a few examples.

ON THE ORDER OF GAUSS-RUNGE-KUTTA METHODS FOR DIFFERENTIAL AND VOLTERRA INTEGRAL EQUATIONS WITH VARIABLE DELAY

Hermann Brunner (Memorial University of Newfoundland, Canada)

Consider the differential equations

$$y'(t) = ay(t) \quad (t \geq 0; y(0) = y_0),$$

and

$$y'(t) = ay(t) + by(t - \tau) \quad (t \geq 0; y(t) = \phi(t), t \leq 0),$$

where a and b are constants; $\tau > 0$ is a constant delay. Let v_n be the approximation to $y(t_n)$ generated by an m -stage implicit RK method that corresponds to collocation by continuous piecewise polynomials of degree m . Suppose that the Volterra integral equations corresponding to the above DEs are solved by collocation in the space of discontinuous piecewise polynomials of degree $m - 1$ ($m \geq 1$), and let u_{it} be the iterated collocation solution based on this collocation solution u . It is well known that

$$\max_{1 \leq n \leq N} |y(t_n) - v_n| = \max_{1 \leq n \leq N} |y(t_n) - u_{it}(t_n)| = \mathcal{O}(h^{2m}),$$

provided the same collocation parameters, namely the Gauss (-Legendre) points, are employed in the computation of v and u .

In this talk we show that these results are no longer true for equations with *variable delay* qt ($0 < q < 1$),

$$(1) \quad y'(t) = ay(t) + by(qt), \quad y(0) = y_0,$$

and

$$(2) \quad y(t) = y_0 + \int_0^t ay(s) ds + \int_0^{qt} (b/q)y(s) ds.$$

In other words, the dynamics of the collocation solution v of (1) (an equation that has been analyzed extensively in recent work by Buhmann and Iserles) is not identical with that of the iterated collocation solution u_{it} of the equivalent integral equation (2).

We will also show that, in spite of this difference, collocation and iterated collocation based on the Gauss points still yield local superconvergence results which, however, are no longer related to the (m, m) -Padé approximant of the analytical solution: the order of local superconvergence on Π_N will now be less than $2m$.

NUMERICAL TREATMENT OF A NON-UNIQUELY SOLVABLE VOLTERRA INTEGRAL EQUATION

Evelyn Buckwar (Freie Universität Berlin, Germany)

In this talk a nonlinear non-uniquely solvable Volterra Integral Equation is considered. The speaker will present an analytical method for obtaining a nontrivial solution. An approximation method derived from the analytical method is introduced, and the results of numerical experiments are demonstrated.

NUMERICAL APPROXIMATIONS OF SOLUTIONS OF RADially SYMMETRIC NONLINEAR ELLIPTIC PDES WITH CRITICALLY GROWING NONLINEARITIES

Chris Budd (University of Bristol) & *Tony Humphries, Andy Wathen* (University of Bristol).

This is the first of two talks in which we study the numerical solution of nonlinear elliptic partial differential equations in three dimensions using piecewise linear finite elements. We will look at problems of the form

$$\Delta u + f(u; \lambda) = 0, \quad u > 0, \quad u|_{\partial\Omega} = 0$$

where the nonlinear function $f(u; \lambda)$ grows rapidly with u . In particular we look at the problem $f(u; \lambda) = \lambda u + u^{5+\epsilon}$ which is important in differential geometry. If Ω is the unit ball and $\epsilon = 0$ then solutions of the PDE exist iff $\lambda > \pi^2/4$. Classical convergence theory shows that if an isolated solution u of the PDE exists then for sufficiently small mesh size h there is a numerical solution U_h such that $\|u - U_h\|_\infty < Bh^2 \log(h)$. In the first talk we will look at symmetric solutions on the unit sphere and will use the technique of matched asymptotic expansions, to derive a sharp convergence theory when $\lambda > \pi^2/4$. This gives an (optimal) estimate of $B = \|u\|_\infty^9/2$. The asymptotic theory is sufficiently descriptive for the numerical solution to be extrapolated to obtain a more accurate answer and an estimate for the value of λ at which solutions cease to exist.

We shall also look at the case of $\lambda \leq \pi^2/4$ and show that (spurious) solutions of the discretisation exist (when the underlying problem has no solution) and will demonstrate that these grow at a rate proportional to $h^{-1/4}$ as the mesh is refined. (This slow rate of growth makes it hard to differentiate between a true and a spurious solution.)

In a subsequent talk (see the abstract of A.R. Humphries) we look at solutions of the PDE on more general three dimensional domains.

MULTIQUADRIC PRE-WAVELETS ON NON-EQUALLY SPACED CENTRES

M.D. Buhmann (ETH Zentrum, Switzerland)

In this talk, prewavelets are discussed that stem from spaces spanned by translates of the multiquadric function and other radial basis functions with non-equally spaced centres. General square-integrable functions can thereby be expanded in series of those prewavelets. Therefore the relatively new theory of (pre-)wavelets which is highly successful

in practice can now be applied in the context of radial basis functions. The purpose of this is to use the good approximation properties of radial basis function spaces (that are well-known and have been discussed at several earlier Dundee conferences) to get new classes of useful prewavelets.

A PARALLEL IMPLEMENTATION OF A DEFLATION ALGORITHM FOR SOLVING LARGE LINEAR SYSTEMS OF EQUATIONS

Kevin Burrage (University of Queensland, Australia) & *Alan Williams* (University of Queensland, Australia).

This paper discusses a new and general iterative technique for solving linear systems of equations. As the iteration process proceeds information is obtained about the eigenvalues of the iteration matrix which either cause slow convergence or divergence. These eigenvalues (and associated eigenvectors) are then deflated into a stiff subspace. This then leads to a coupled iteration process between the underlying iteration on the non-stiff space and a Newton iteration on the (small) stiff system. This process can rapidly accelerate the convergence of any iterative scheme.

Numerical results are presented which show the efficacy of this approach. Finally, some numerical results are presented for a parallel implementation on the INTEL Paragon for large linear systems arising in the area of environmental modelling. These problems arise from the fitting of a thin plate smoothing spline to noisy rainfall data (collected within Australia) using the minimization of the Generalized Cross Validation (GCV) function.

NUMERICAL SOLUTION TO TWO-PHASE STEFAN PROBLEMS BY THE HEAT BALANCE INTEGRAL METHOD

J. Caldwell (University of Hong Kong) & *C.K. Chiu* (University of Hong Kong).

Caldwell and Chiu have used the heat balance integral method to solve one-phase solidification problems. In this talk the method is extended to two-phase Stefan problems that arise when the effect of sub-cooling is taken into consideration. Numerical results for the two-phase cylindrical problem are obtained for a range of sub-divisions, sub-cooling parameters, Stefan number and ratio of conductivities. The effects of variation of parameters on the solidification process are also studied.

CONTROLLED CHOLESKY FACTORISATION FOR PRECONDITIONING THE CONJUGATE GRADIENT METHOD

Frederico F. Campos (University of Oxford and Universidade Federal de Minas Gerais, Brazil) & *John S. Rollett* (University of Oxford (in memoriam)).

The controlled Cholesky factorisation is based on minimisation of the Frobenius norm of $L - G$, where L and G are the complete and incomplete factors of the coefficient matrix, respectively. This minimisation is made by allowing more fill-in using a pre-set value η and selecting only the largest elements by column. The sparsity pattern of the original matrix is ignored and storage required is easily predictable. Also, a reliable scheme is used to avoid loss of positive definiteness. Performance of the Controlled Cholesky Conjugate Gradient method, CCCG(η), is presented, showing that CCCG(0) has better performance than ICCG(0) since a more suitable eigenspectrum is produced.

GAUSSIAN SYMMETRIZERS APPLIED TO INDEX-2 DIFFERENTIAL-ALGEBRAIC EQUATIONS

R.P.K. Chan (University of Auckland, New Zealand)

Gauss methods are not appropriate for the numerical solution of differential-algebraic equations of index 2. However, certain compositions based on Gauss methods, called Gaussian symmetrizers, which preserve symmetry in the sense of h^2 -asymptotic error expansions can give L -stable methods which can be appropriate. In this talk we discuss the construction of symmetrizers based on Gauss methods with 2 and 3 stages, and present some test results for a method of order 5 for both the differential and algebraic components.

A COMPOSITION LAW FOR RUNGE-KUTTA METHODS APPLIED TO INDEX-2 DIFFERENTIAL-ALGEBRAIC EQUATIONS

P. Chartier (IRISA, Campus de Beaulieu, France)

This talk presents a new composition law for Runge-Kutta methods when applied to differential-algebraic systems. Applications of this result to the study of the order of composite methods and of symmetric methods will be given.

ON THE STABILITY OF LOD DIFFERENCE SCHEMES WITH RESPECT TO BOUNDARY CONDITIONS

Raimondas Čiegis (Institute of Mathematics and Informatics, Lithuania)

We consider the following Locally One Dimensional scheme

$$\begin{aligned} y_{\bar{t}_\alpha} &= \Lambda_\alpha 0.5(y_\alpha + y_{\alpha-1}) + \psi_\alpha, \quad \alpha = 1, 2, \dots, p, \\ y_\alpha &= g_\alpha, \quad (x, t) \in \gamma \times \omega_r, \\ y(0) &= u_0(x), \quad y(t_{j+1}) = y_p, \end{aligned}$$

where Λ_α is a standard finite-difference approximation of the one-dimensional second order differential operator and g_α, ψ_α are the boundary conditions and the source term approximations, respectively. We also consider the symmetric LOD scheme, where symmetry can be restored by interchanging the direction of splitting after each step.

New stability estimates with respect to boundary conditions are proved. These results are used to investigate the accuracy of LOD schemes when no special boundary correction technique is used for the realization of LOD schemes. The accuracy of LOD schemes with first-order boundary correction terms is also investigated.

A CLOSE LOOK AT EFM5, A CODE BASED ON SIXTH-ORDER EXPONENTIAL-FITTED METHODS IN FIVE POINTS FOR SOLVING $y'' = f(x, y)$

M. Van Daele (Universiteit Gent, Belgium) & *L. Gr. Ixaru, G. Vanden Berghe and H. De Meyer* (Universiteit Gent, Belgium).

There is a considerable interest in deriving exponential-fitted multistep methods for $y'' = f(x, y)$, but most of the efforts were mostly concentrated on the particular case of a single equation with a linear homogeneous form for $f(x, y)$, viz. $f(x, y) = g(x)y$. In fact, the literature covers almost exclusively the solution of the Schrödinger equation and of the Sturm-Liouville problem. The achievements reported were impressive enough to look for extension towards systems of equations with non-linear expressions for $f_i(x, y_1, \dots, y_n)$. We will discuss the sixth-order code EFM5, based on four-step exponential-fitted methods for which the classical counterparts constitute a one-parameter family which makes these

methods very attractive from a practical point of view: this property makes it possible to autonomously generate the extra starting values when two of them are given as input and also to halve or double the step size during the integration.

Without going into the very details, the talk will be concentrated on some general ideas that have been used in this code: how to obtain the weights of such exponential-fitted methods, how to fit the values of the parameters in the input exponentials in terms of the form of $f(x, y)$, how to start the integration, how to change the stepsize, what about stability, etc. Finally, a comparison is made for a few examples with the very popular code seventh-order code DOPRIN. It will be shown that our algorithm is highly competitive, expecially when high accuracies are required.

RECURSIVE PROJECTION FOR SEMI-LINEAR PDE

Bryan Davidson (Aspentech UK Ltd)

A recursive projection method for a class of semi-linear PDE is presented. The spectral dominance of the linear part is exploited to achieve an efficient splitting. The resulting algorithm will perform numerical continuation and detect steady state and Hopf bifurcation without forming and postprocessing Jacobian matrices. The results of some numerical experiments are presented.

INSTABILITIES IN MIXED FINITE ELEMENT APPROXIMATIONS OF TIME DEPENDENT BOUNDARY INTEGRAL EQUATIONS

Penny J. Davies (University of Dundee)

Mixed finite element approximations of time dependent boundary integral equations (of the type used to compute the current induced on a perfect conductor by an incident electric pulse) are often observed to be numerically unstable. We show how Fourier analysis can be used to identify fast growing unstable modes, and describe how they can be removed by applying an appropriate spatial filter to the solution. These modes seem to be caused by a combination of the basis functions and the quadrature rule used for the integral equations, and do not appear to be present when similar finite element approximations are used for the wave equation.

INCOMPLETE MULTILEVEL FACTORIZATIONS

J.C. Díaz (University of Tulsa, U.S.A.) & *M. Komara* (University of Tulsa, U.S.A.).

We discuss the extension of ILU factorizations to multilevel systems generated from self-adjoint PDEs. The resulting incomplete multilevel factorization is shown to be spectrally equivalent to the ILU of the composite multilevel matrix. The application of the incomplete multilevel LU is achieved via a V-Cycle. The multilevel factorization requires nearly half the operations of the inexact BEPS preconditioner. Representative results illustrate the potential of the method. [Research partly supported by Oklahoma Center for Advancement of Science and Technology Grants RB9-008 (3748) and ARO-36 (3910).]

NUMERICAL SOLUTION OF A SINGULAR VOLTERRA INTEGRAL EQUATION

Teresa Diogo (Instituto Superior Técnico, Portugal) & *Neide Bertoldi Franco* (ICMSC - USP de São Carlos, Brazil).

This work is concerned with the numerical solution of a certain Volterra integral equation with weakly singular kernel. We introduce a class of product integration methods with arbitrary orders of convergence, under the assumption that the exact solution is sufficiently smooth, thus generalising the results of previous work. Some numerical examples are presented which illustrate the theoretical estimates obtained.

NUMERICAL STABILISATION OF THE MULTIDIMENSIONAL NEWTON METHOD FOR NON-LINEAR PROBLEMS

M. Drexler (Oxford University) & *I.J. Sobey* (Oxford University).

We propose a modified version of Newton's method that shows improved stability and can be used as a global solver for nonlinear problems arising from the discretisation of partial differential equations. The method relies on a restricted step approach for the Newton shifts using various control mechanisms to avoid local minima and regions of Jacobian singularity. In the first steps of the convergence history, stability is gained at the price of linear convergence by perturbing the Jacobian where necessary. These perturbations are relaxed in the later steps, thus gradually returning to the original Newton method with its desirable local convergence properties. The proposed method is capable of dealing with functions where the range for some of the variables is restricted, as arising in many physical problems.

We present a convergence analysis for the modified Newton method and point out several of the complications that can arise from stiff problems and their possible remedies. As many of the problems are related to specially structured Jacobians, we devote particular interest to the stable solution of linear systems. A geometrical interpretation of the modified Newton method in multiple dimensions is given and compared with that of the original method.

The performance of the algorithm is shown for several test problems in one and multiple dimensions. As an example of a physical problem, we use the model problem of steady-state turbulent flow in a parallel channel. The $k - \epsilon$ turbulence equations are discretised on a two-dimensional MAC mesh using finite differences with mixed upwinding and central differencing. The solution is computed for various Reynolds numbers and initial conditions to demonstrate the stability of the modified Newton method.

OVERLAPPING GRIDS AND WAVE EQUATIONS

Dugald B. Duncan (Heriot-Watt University)

Computer simulation of linear wave propagation has applications in areas including ultrasonic testing, seismology and electromagnetic scattering. Realistic problems often involve modelling the wave interactions with collections of small objects aligned in different ways, such as cracks or inclusions in rock structures. High accuracy difference schemes for linear wave problems exist, but usually require a uniform grid, and this does not fit the geometry of most problems.

We examine the use of overlapping grids in wave problems, where cracks and inclusions are embedded in their own local uniform grids which overlay a uniform underlying grid. Information is passed between grids by interpolation. We analyse some simple representative cases and illustrate results obtained in the solution of acoustic and elastic (forward) scattering problems involving multiple cracks and inclusions with arbitrary locations and orientations.

RECENT DEVELOPMENTS IN THE EVALUATION OF IRREGULAR OSCILLATORY INTEGRALS

G. A. Evans (De Montford University)

In numerical quadrature, the classic problems which are not resolved by general purpose methods such as those of Gauss, Clenshaw-Curtis and Patterson, are those which have singular or oscillatory integrands. Oscillatory forms of the regular type $\int_a^b f(x) \frac{\sin}{\cos} \omega x dx$ are well understood and will be only briefly surveyed. Many physical problems such as

water wave computations give rise to irregular problems of the form $\int_a^b f(x) \frac{\sin}{\cos} \omega q(x) dx$ for which quite different techniques from the regular case are needed. These are the subject of some very recent research in quadrature, which will be covered in this presentation. The work includes extensions to Bessel function oscillations and to semi-infinite range problems which have applications in the numerical inversion of transforms and in problems with combinations of singular and oscillatory integrands.

RELIABLE AND ACCURATE SOFTWARE FOR EVALUATING COMPLEX ELEMENTARY FUNCTIONS

Thomas F. Fairgrieve (University of Toronto, Canada) *T. E. Hull* (University of Toronto, Canada) & *Ping Tak Peter Tang* (Argonne National Laboratory, U.S.A.).

The state of the art in the evaluation of real-valued elementary functions has advanced to the stage that good-quality, portable software is freely available. The same cannot be said about the case of complex-valued elementary functions. It is not difficult to find faults in software currently distributed by some computer manufacturers and numerical library producers. The delay in the development of robust software for this problem is due to the fact that there are many numerical pitfalls lurking in the straightforward evaluation of formulas for the complex elementary functions. These pitfalls can lead to spurious arithmetic exceptions and also cancellation difficulties.

We have developed reliable and accurate algorithms for the evaluation of the complex functions required by Fortran, namely, *cabs*, *csqrt*, *cexp*, *clog*, *csin* and *ccos*, and also the complex inverse trig functions *arcsine*, *arccosine* and *arctangent*. The algorithms use a convenient exception-handling construct. The algorithms will be presented, together with error bounds on their results.

A POSTERIORI ERROR ESTIMATES FOR SEMILINEAR ELLIPTIC EQUATIONS WITH APPLICATIONS TO THE SEMICONDUCTOR EQUATIONS

R.C. Ferguson (University of Bath)

We present a posteriori error estimates of Eriksson and Johnson type for a class of semilinear elliptic equations in 1 and 2 dimensions. Our estimate bounds the error in the finite element solution in terms of a suitable residual norm and can be used as one component in an adaptive strategy for finite element approximation. We test such an adaptive scheme on a model 1D singularly perturbed Poisson-Boltzmann equation arising in semiconductor device modelling. We show numerical results, which demonstrate that the adaptive method is capable of calculating the width of the depletion layer in a p-n diode up to the correct order of dependence on the singular perturbation parameter (which is known from singular perturbation theory).

STABLE NULL SPACE FACTORS FOR KKT SYSTEMS

R. Fletcher (University of Dundee) & *T. Johnson* (University of Dundee).

The calculation of a null space matrix by direct elimination, followed by the factorization of a reduced Hessian matrix, is a key technique in large scale quadratic programming. It is observed that this technique also can provide a method for factorizing a KKT matrix

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

such as arises in many fields. The factorization may be implemented in two different ways. When A is close to being rank deficient, it is shown that one method is quite

stable, whereas the other is not. The reasons for this are outlined. The phenomenon is confirmed by a range of experiments in Matlab. Some error analysis is presented.

STABILITY OF A NUMERICAL SOLUTION OF A NON-LINEAR VOLTERRA INTEGRAL EQUATION OF CONVOLUTION TYPE

Neville J Ford (Chester College)

We consider the use of certain classes of quadrature rule in the numerical solution of

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

We derive conditions under which the qualitative behaviour of the solution to the integral equation is preserved in the numerical scheme.

A PSEUDOSPECTRAL APPROACH FOR POLAR AND SPHERICAL GEOMETRIES

B. Fornberg (University of Colorado, U.S.A.)

Pseudospectral (PS) methods have proven to be far more cost-effective than finite differences (FD) or finite elements (FE) in many applications that feature simple domains, which allow the use of highly regular computational grids (such as rectangles etc.). The principal difficulty with a spherical domain is that it is impossible to cover its surface with a grid that is both uniform and dense (i.e. denser than the 20 corners of the icosahedron). The main previous approaches to reach high accuracies have been:

- Use of approximately uniform grids (like the dimple pattern on a golf ball—however, this is algebraically too complex for all but low order FD or FE methods),
- Use of spherical harmonics (highly accurate, but again algebraically complex as well as numerically slow due to the lack of a fast Legendre transform technique - this approach has still proven competitive in areas such as meteorology and astrophysics),
- Use of FD or Fourier approximations along latitude lines together with FD or Chebyshev PS approximations along longitude lines (leading to several types of ‘pole problems’).

Viewing PS methods as limiting cases of FD methods (as their orders of accuracy tend to infinity) leads to a new class of very simple, yet highly effective entirely FFT-based PS methods, which turn out to bypass the previously encountered ‘pole problems’.

EFFICIENT USE OF THE NONLINEAR GALERKIN METHOD

Bosco García Archilla (Universidad Autónoma de Madrid, Spain) *Julia Novo* (Universidad de Valladolid, Spain) & *Edriss S. Titi* (University of California at Irvine, U.S.A.).

Nonlinear Galerkin methods (NLG) [2] are novel ways of discretizing dissipative PDEs that have attracted a great deal of attention in recent years. One of their main advantages is that they present higher convergence rates than classical Galerkin methods. However, some recent numerical studies [1], [3] show that their superior accuracy is obtained at a big computational cost, making them less effective than classical methods. Hence, from the computational point of view, it is not clear that NLG methods represent an improvement over classical Galerkin methods.

In the present paper, a novel method, based on the ideas of the NLG is introduced.

Numerical tests show that its rate of convergence is that of the (more accurate) NLG, but its computational cost is that of the (cheaper) classical Galerkin. The analysis of the new method is also presented.

- [1] B. García-Archilla & J. de Frutos, Time integration of the non-linear Galerkin method, *IMA J. Numer. Anal.* **15**, 221–244, 1995.
- [2] M. Marion & R. Temam, Nonlinear Galerkin methods, *SIAM J. Numer. Anal.* **26**, 1139–1157, 1989.
- [3] R. Wallace & D. Sloan, Numerical solutions of a non-linear dissipative system using a pseudospectral method and inertial manifolds, (to appear in *SIAM J. Sci. Comput.*).

STABILITY OF TIME-STEPPING METHODS FOR ABSTRACT QUASILINEAR PARABOLIC PROBLEMS

Cesareo Gonzalez (Universidad de Valladolid) & *C. Palencia* (Universidad de Valladolid).

We consider time discretizations of quasilinear parabolic problems. We work in the Banach spaces setting, so that non-Hilbert norms, like the L^p , $p \neq 2$, norms, are allowed in our study. The continuous problem being analyzed is the form

$$(1) \quad u'(t) = A(u(t)), \quad t \in I, \quad \text{with} \quad u(t_0) = u_0 \in D(A(u_0)),$$

where $I \subset \mathbb{R}$ is an interval, $A(u) : D(A(u)) \subset X \rightarrow X$, $u \in V$ open set in X , is a family of linear operators with dense domains fix $D = D(A(u))$. The assumptions on the problem are similar to classical hypotheses in the study of abstract quasilinear parabolic problems. Roughly speaking, we suppose that (i) the frozen problems obtained from (1), i.e. the initial value problems associated with $A(u^*)$, for each u^* fixed in V , are parabolic and (ii) the dependence of the operators $A(u)$ with respect to u is Lipschitz with respect to some suitable interpolation spaces between D and X . Problem (1) is discretized in time by a Runge-Kutta method. As far as the numerical method is concerned, our basic assumption is the $L(\theta)$ -stability of the method, for some angle $\theta \in (0, \pi/2]$. The main result to present communication establishes the stability of such discretization of (1).

A MULTIGRID-TYPE METHOD FOR THIN PLATE SPLINE INTERPOLATION ON A CIRCLE

George Goodsell (University of Cambridge)

We consider the problem of thin plate spline interpolation to n equally spaced points on a circle, where the number of data points is sufficiently large for work of $\mathcal{O}(n^3)$ to be unacceptable. We adopt an iterative multigrid-type method, each iteration comprising n_{grid} stages, and n being an integer multiple of $2^{n_{grid}-1}$. We let the first grid, V_1 , be the full set of data points, V , and each subsequent (coarser) grid, $V_2, V_3, \dots, V_{n_{grid}}$, contain exactly half of the data points of the preceding (finer) grid, these data points being equally spaced.

At each stage of the iteration, we correct our current estimate of the thin plate spline interpolant by an estimate of the interpolant to the current residuals on V_k , but which is calculated using Lagrange functions of interpolation, each of which is constructed from only a *small local subset* of p data points in V_k . When the coarsest grid is reached, however, then the interpolation problem is solved exactly on its $q = n/2^{n_{grid}-1}$ points. The iterative process continues until the maximum residual does not exceed a specified tolerance.

Each iteration has the effect of premultiplying the vector of residuals by an $(n \times n)$ matrix

R , and thus convergence will depend upon the size of the spectral radius, $\rho(R)$, of this matrix. We investigate the dependence of the spectral radius on the values of n , p , and q . In all the cases we have considered, we find $\rho(R) \ll 1$, and thus rapid convergence is assured.

APPROXIMATE INVERSE PRECONDITIONERS FOR NONSYMMETRIC LINEAR SYSTEMS

N. I. M. Gould (Rutherford Appleton Laboratory) & *J. A. Scott* (Rutherford Appleton Laboratory).

In this talk, we consider preconditioning the iterative solution of nonsymmetric linear systems $\mathbf{A}\mathbf{x} = \mathbf{b}$ using approximations $\mathbf{M}$ to the inverse of $\mathbf{A}$. Based on existing work, we construct approximations to $\mathbf{A}^{-1}$ by solving the problem

$$\begin{aligned} &\text{minimize } \|\mathbf{A}\mathbf{M} - \mathbf{I}\|_F^2, \\ &\mathbf{M} \in \mathcal{M} \end{aligned}$$

where $\mathcal{M}$ is a predefined sparsity pattern. This problem decomposes into n independent least-squares subproblems

$$\begin{aligned} &\text{minimize } \|\mathbf{A}\mathbf{m}_i - \mathbf{e}_i\|_2^2, \\ &\mathbf{m}_i \in \mathcal{M}_i \end{aligned}$$

thus offering considerable scope for parallelism. We show how these subproblems may be solved efficiently as we increase the allowed sparsity pattern $\mathcal{M}_i$, and consider a number of variations which aim to improve the effectiveness of the overall method. We conclude by comparing these techniques with other preconditioning schemes.

BEST APPROXIMATION BY PERFECT SPLINES WITH END CONDITIONS

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

In this paper we shall analyse the problem of the best approximation of an element of a seminormed Sobolev space, $K^r[a, b]$, in the linear space $\text{GPS}(\Delta; 2r - 1, Q)$, $Q = \{q_0, q_1, \dots, q_n\}$, $\Delta = \{x_j\}_{j=1}^n$, (whose dimension we determine), of the polynomial perfect splines of degree $2r - 1$ and continuity q_j on x_j , satisfying the end conditions

$$\begin{cases} s^{(\alpha)}(x_0) = 0 & \alpha = r, r + 1, \dots, q_0 \\ s^{(\beta)}(x_n) = 0 & \beta = r, r + 1, \dots, q_n \end{cases}.$$

The existence and uniqueness of an interpolating best approximation on x_j , $j = 1, 2, \dots, n$, also analysed.

A NEW METHOD FOR THE ACCELERATION AND CONVERGENCE OF A SEQUENCE OF VECTORS

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

Given a sequence of vectors $\underline{s}_0, \underline{s}_1, \underline{s}_2, \dots$ with $\underline{s}_j \in C^d$ or R^d and $\underline{s}_n \rightarrow \underline{s}_\infty$ as $n \rightarrow \infty$, linear combinations of vectors $\underline{s}_i$ can be found which, under suitable conditions, converge to $\underline{s}_\infty$ more quickly than the original sequence. Sequences of this kind occur frequently in the numerical solution of PDEs by discretisation. An approach to this problem using orthogonal polynomials and its connection with Lanczos methods is well known. A similar approach, which works well in principle but less well in practice, is based on the vector epsilon algorithm. In this talk, we will discuss a new method in which a polynomial

accelerator is constructed.

It evolved from the vector epsilon algorithm in an attempt to mitigate the drawbacks of VEA. It appears likely that this polynomial accelerator is identical, in principle, to Roberts' method based on vector-valued functions.

DATA ASSIMILATION IN NUMERICAL WEATHER PREDICTION USING CONTROL THEORY
A. K. Griffith (University of Reading) & *N. K. Nichols* (University of Reading).

Data assimilation provides a means for combining observational data with numerical weather prediction models, in order to improve the estimate of the atmospheric state. We will present a brief comparison of various data assimilation techniques with particular attention given to a data assimilation scheme based on optimal control theory. The aim in this case is to minimize a cost functional expressing the distance between the model state and the observations, subject to the constraint that the model equations still hold. This huge optimisation problem is solved iteratively using a descent method and adjoint models to find the gradients required in the minimization. An important issue at present is how we can allow for model error in the data assimilation process, and this will also be discussed.

ON THE EXTENSION TO 2-D LEAST ORDER POLYNOMIAL REALISATION OF A T.F. MATRIX

M.L. Hadji (Universite de Annaba, Algeria)

2-D polynomial system matrices which arise, following different situations, from e.g. high order partial differential equations or retarded delay differential systems play a fundamental role in describing controllability and observability properties of the above systems. In this work, we try to extend Rosenbrock's result on the characterisation of all least order polynomial realisations of a T.F. matrix from 1-D to 2-D systems using MC and ZC concepts.

AN ASYNCHRONOUS PARALLEL ALGORITHM FOR THE REVISED SIMPLEX METHOD

J. A. J. Hall (University of Edinburgh) & *K. I. M. McKinnon* (University of Edinburgh).

Hall and McKinnon are developing parallel algorithms for the revised simplex method in which one master processor is dedicated to inverting basis matrices and the remaining n worker processors perform simplex iterations. These are overlapped as much as possible whilst still following a single path. A synchronous algorithm has been implemented on a Cray T3D, with each processor performing every n^{th} iteration in a fixed sequence. Inefficiencies due to duplication of work, communication overheads and idleness resulting from the use of out-of-date prices lead to only a modest improvement in performance over that of a serial implementation. The issue of efficiency has been investigated with a synchronous code which follows a pre-defined sequence of basis changes and now achieves a significant speed-up. The problems associated with idleness in the synchronous parallel solver have led to the development of an asynchronous algorithm with which it is expected to achieve worthwhile speed-up.

ERRORS OF LINEAR INTERPOLATION ON A TRIANGLE

D.C. Handscomb (University of Oxford)

We attempt to determine best possible bounds for the errors in function value and gradient when a bivariate function is approximated by linear interpolation between values at the vertices of a triangle of known shape and size. We consider both L_2 and L_∞ bounds, in terms of L_2 and L_∞ measures of smoothness of the function.

AN ALTERNATIVE FINITE-DIFFERENCE METHOD APPLIED TO THE SAL'NIKOV OSCILLATOR PROBLEM

Udo S. Herges (Brunel University) & *E.H. Twizell* (Brunel University).

Replacing the derivatives in a system of differential equations by first-order finite differences and then iterating the difference equations is common practice to calculate numerical solutions to the system. Going on step further, not only the derivatives are approximated, but also the dependent variables themselves can be replaced by order-consistent differences involving parameters. The resulting numerical schemes are, in general, implicit but the parameters may be chosen in such a way as to obtain an explicit computation scheme which retains the superior stability properties of implicitness.

This alternative finite-difference method is derived for, and applied to the Sal'nikov thermokinetic oscillator problem, a highly nonlinear, two-dimensional, initial-value problem, modelling a sequence of chemical reactions.

TIME-STEPPING AND PRESERVING ORTHOGONALITY

Desmond J. Higham (University of Dundee)

Certain applications produce initial value ODEs whose solutions, regarded as time-dependent matrices, preserve orthogonality. One such application arises in the computation of Lyapunov exponents.

For some special problem classes, there exist time-stepping methods that automatically inherit the orthogonality preservation. However, a more widely applicable approach is to apply a standard integrator and regularly replace the approximate solution by an orthogonal matrix. Usually, the approximate solution is replaced by the factor Q from its QR decomposition. (This can be done, for example, by using the modified Gram-Schmidt algorithm.) However, the optimal replacement—the one that is closest in the Euclidean or Frobenius norm—is given by the orthogonal polar factor. A quadratically convergent algorithm (the Schultz iteration) can be used to compute this factor. Hence, we argue that perturbing towards the orthogonal polar factor is a natural choice. Further, the “optimality” property allows us to prove that the perturbations do not degrade the finite-time global error bound for the ODE solution. Finally, using a recent result of Ji-guang Sun, we show how the global error bound carries through to the more usual case where the orthogonal QR factor is used instead of the orthogonal polar factor.

STABILITY OF THE DIAGONAL PIVOTING METHOD WITH PARTIAL PIVOTING

Nicholas J. Higham (University of Manchester)

LAPACK and LINPACK both solve symmetric indefinite linear systems using the diagonal pivoting method with the partial pivoting strategy of Bunch and Kaufman (1977). No proof of the stability of this method has appeared in the literature. It is tempting to argue that the diagonal pivoting method is stable for a given pivoting strategy if the growth factor is small. We show that this argument is false in general, and give a sufficient condition for stability. This condition is not satisfied by the partial pivoting strategy, because the multipliers are unbounded. Nevertheless, using a more specific approach we are able to prove the stability of partial pivoting, thereby filling a gap in the body of theory supporting LAPACK and LINPACK.

OPERATOR BOUNDS FOR A POSTERIORI ESTIMATES

A. T. Hill (Bath University)

Let $(Au)(x) = -a_{ij}(x)D_iD_ju + b_i(x)D_iu$ for $u \in H^2(\Omega) \cap H_0^1(\Omega)$, where bounded $\Omega \subset \mathbb{R}^N$. Suppose that for all $x \in \Omega$ we impose the constraints $a_{ij}(x)\xi_i\xi_j \geq |\xi|^2$ for all $\xi \in \mathbb{R}^N$ and $|b_i(x)| \leq M$. Then, considering A^{-1} as an operator in $L_p(\Omega)$, we present sharp estimates for the smallest eigenvalue, $\|A^{-1}\|_p$, $\|e^{-At}\|_p$ and $\|(\lambda I + A)^{-1}\|_p$, $\lambda > 0$.

Considerations include the relevance to a posteriori estimation; the physical significance and the computational ill-posedness of the worst case, i.e. when $\|A^{-1}\|_p$ is largest; the regularisation of $\|(\lambda I + A)^{-1}\|_p$ when $\lambda > 0$; the universal well-posedness of the parabolic problem; the worst possible ‘hump’ behaviour of $\|e^{-At}\|_2$, in the sense of Trefethen; the astronomically slow decay of some parabolic problems; indications that the ‘worst case’ is untypical.

ADAPTIVE LAGRANGE-GALERKIN METHODS FOR UNSTEADY CONVECTION-DIFFUSION PROBLEMS

P. Houston (Oxford University) & **E. Süli** (Oxford University).

The modelling of convection-diffusion processes is a central problem in many fields, particularly fluid dynamics. Typically, the solutions to these problems exhibit very isolated phenomena, such as internal and boundary layers. In order to resolve these features accurately, with the minimum computational effort, it is desirable to use adaptively refined meshes.

We shall focus on adaptivity for the Lagrange-Galerkin finite element method. The Lagrange-Galerkin method combines the method of characteristics with the standard Galerkin finite element method. The method is designed for the simulation of time-dependent convection (dominated) diffusion problems. The advantages of the method are its high accuracy and good stability properties.

In this paper we derive an a posteriori error estimate in the $L^2(L^2)$ -norm for the Lagrange-Galerkin discretisation of the unsteady two-dimensional convection-diffusion problem. The proof of the error estimate is based on so-called strong stability estimates for an associated backward dual problem, together with the Galerkin orthogonality of the finite element method. Based on this a posteriori error estimate, we design an adaptive algorithm for determining both the space and time discretisation parameters in such a way as to yield *global* error control in the $L^2(L^2)$ -norm with respect to a pre-determined tolerance, TOL.

THREE-DIMENSIONAL TRANSPORT OF POLLUTANTS IN SHALLOW SEAS

P. J. van der Houwen (CWI, The Netherlands)

In three-dimensional numerical modelling of transport of pollutants in Shallow Seas, we may distinguish three phases: (i) the development of a (three-dimensional) hydrodynamical model, (ii) the development of a (three-dimensional) transport model, and (iii) the coupling of the transport model with an ecological or biochemical model. In this talk, we discuss phases (ii) and (iii). The complete model consists of a system of k coupled partial differential equations for the concentrations $c_1, \dots, c_k$ of the k pollutants of the form

$$\frac{\partial c_i}{\partial t} = L(\mathbf{v})c_i + g_i(x, y, z, t, c_1, \dots, c_k), \quad i = 1, \dots, k.$$

Here $\mathbf{v}$ denotes the three-dimensional fluid velocity field, L is the convection-diffusion operator in the spatial coordinates x, y and z , and the functions g_i describe the chemical

reactions and the emissions from sources. The velocity field $\mathbf{v}$ is assumed to be provided by the hydrodynamical model. The numerical model will be based on splitting methods that are only implicit in the vertical spatial direction. This approach enables us to apply domain decomposition without any difficulties of matching the various domains. As a consequence, the resulting algorithm is highly parallel and allows for large scale simulations.

NUMERICAL APPROXIMATIONS OF SOLUTIONS FOR SEMI-LINEAR ELLIPTIC PDEs WITH CRITICAL SOBOLEV EXPONENTS ON NON-SPHERICAL 3D DOMAINS

A.R. Humphries (University of Bristol) & *C.J. Budd, A.J. Wathen* (University of Bristol).

As in the preceding talk (by C.J. Budd) we consider problems of the form

$$\Delta u + f(u; \lambda) = 0, \quad u > 0, \quad u|_{\partial\Omega} = 0$$

where $\Omega \subset \mathbb{R}^3$ is bounded, and the nonlinear function is critical: in particular we consider $f(u, \lambda) = \lambda u + u^5$. Much is known about the radially symmetric case (for then the problem reduces to a scalar ODE). We consider general solutions on nonspherical domains, beginning initial with cuboid domains, and compute numerical solutions using the Finite Element Method together with path following in λ . We work with relatively fine meshes ($\approx 10^6$ nodes) which necessitates use of an approximate Newton iteration to solve the nonlinear FEM equations (it is infeasible to store the Jacobian), and we use the Conjugate Gradient method to compute the Newton updates.

We wish to calculate the value λ_0 at which solutions cease to exist, but as in the radial case find that spurious numerical solutions exist for $\lambda < \lambda_0$. Under mesh refinement these spurious solutions become unbounded in $L^\infty(\Omega)$ but at a rate that is so slow that even on the finest meshes we can use it is not possible to distinguish the spurious from the convergent solutions. However we find that the behaviour of the numerical solutions is very similar to the radial case considered in the previous talk, and we use the asymptotic theory presented there to obtain more accurate solutions and estimates for λ_0 .

THREE-DIMENSIONAL STEADY FLOW IN A DIVIDING CHANNEL

Roland Hunt (University of Strathclyde)

A numerical solution for the flow of a steady incompressible fluid in a general symmetric three-dimensional bifurcation having uniform thickness is presented for Reynolds number up to 100. The physical region is divided into three sub-domains, each of which is transformed onto a rectangular parallelepiped upon which the calculations are made. The Navier-Stokes equations are differenced using standard second order differences in the direction of each tube and pseudospectral differences in the two transverse directions. The use of such differences in the transverse plane greatly reduces the number of nodes required for a given accuracy, and this particular mix of differences minimises the CPU time requirement when Newton's method is used to solve the resulting algebraic system. Two bifurcations have been considered with daughter tubes angled to the main tube at 60 and 90 degrees respectively. By comparing results on different sized grids the estimated relative accuracy is typically of order 0.001. The resulting flows display novel three-dimensional features not present in two-dimensional flows. In particular, as fluid passes from main to daughter tubes it twists in a fairly complex vortex-like fashion.

EFFICIENT USE OF ITERATED PENALTY METHOD FOR NAVIER-STOKES EQUATIONS

Andrew Ilin (University of Houston, U.S.A.) & *Babak Bagheri, Ridgway Scott, Ralph Metcalfe* (University of Houston, U.S.A.).

High-order finite element methods provide efficient ways to model complex physical phenomena such as incompressible fluid flows, which are described by the Navier-Stokes Equations. We present some results obtained with high-order finite-element methods for 2-D and 3-D problems using the Iterated Penalty Method. This method reduces the number of unknowns and produces a solution which exactly satisfies the incompressibility condition. For a wide range of penalty parameter values, even one iteration is enough to get solutions (pressure and velocity) with needed accuracy, using a good initial guess coming from the previous time-step. For high-degree finite elements, the Iterated Penalty Method with less than three iterations is computationally cheaper than using the Taylor-Hood method. The method is robust with respect to the value of penalty parameter. An error estimator is constructed that indicates areas of high computational error and is used for the generation of optimal meshes. The numerical experiments were conducted for problems with known analytical solution, like Jeffrey-Hamel flow and also for the problem of flow around a cylinder.

SOBOLEV-ORTHOGONAL FUNCTIONS AND SPECTRAL METHODS FOR PARABOLIC PDES

A. Iserles (University of Cambridge) *M.D. Buhmann* (ETH Zentrum, Switzerland) *Syvart Nørsett* (University of Trondheim, Norway) & *Chus Sanz-Serna* (Universidad de Valladolid, Spain).

The theme of this talk is the solution of the multivariate diffusion equation with a variable diffusion coefficient,

$$\frac{\partial u}{\partial t} = \nabla(a(\mathbf{x})\nabla u) + b(\mathbf{x})u, \quad \mathbf{x} \in \mathcal{V},$$

accompanied by zero Dirichlet boundary conditions. $\mathcal{V}$ is a cube in $\mathbb{R}^d$.

We represent the numerical solution as

$$u(\mathbf{x}, t) = \sum_{\ell=1}^m \alpha_{\ell}(\mathbf{x}) w_{\ell}(t),$$

discretize in space with Galerkin and solve the resultant ODEs with backward Euler (all implicit multistep methods admit similar analysis).

Theorem: Suppose that $\{w_1, w_2, \dots, w_m\}$ are orthogonal with respect to the Sobolev inner product

$$\langle f, g \rangle = \int_{\mathcal{V}} (1 - \Delta t b(\mathbf{x})) f(\mathbf{x}) g(\mathbf{x}) d\mathbf{x} + \Delta t \int_{\mathcal{V}} a(\mathbf{x}) \nabla f(\mathbf{x}) \nabla g(\mathbf{x}) d\mathbf{x}.$$

Then the (implicit!) backward Euler can be written explicitly, without the need to solve any linear algebraic system.

Obvious candidates for the Sobolev-orthogonal basis are polynomials or splines, but both run into severe problems. Instead, we have used a basis of translates of a function. It is possible to prove that for every $a > 0$ and b there exists a function whose translates are dense and orthogonal with respect to the underlying Sobolev inner product. Moreover, such a function can be constructed by using FFT. Our analysis uses concepts from the theory of wavelets.

A SINC QUADRATURE SUBROUTINE FOR CAUCHY PRINCIPLE VALUE INTEGRALS

Patrick Keast (Dalhousie University, Canada) & *Bernard Bialecki* (University of Kentucky, U.S.A.).

This talk will describe the construction of a subroutine for the automatic evaluation of Cauchy principal value integrals. Based on a truncated sum of a Sinc function series, with the function evaluated at shifted Sinc points, the subroutine returns an approximation to the integral together with an estimate of the absolute error. Numerical results demonstrate that the new method works well on functions with singularities.

WAVEFORM RELAXATION METHOD WITH TOEPLITZ OPERATOR SPLITTING

Sigitas Keras (University of Cambridge)

In this talk we consider a waveform relaxation method for the equation

$$\frac{du}{dt} + Au = f, \quad u(0) = u_0$$

in a form

$$\frac{du^{n+1}}{dt} + Pu^{n+1} = Qu^{n+1} + f, \quad A = P - Q,$$

where P is Toeplitz or block Toeplitz matrix. We show that under suitable conditions this method converges. We apply this result for linear parabolic equations with variable coefficients. In this case the rate of convergence can be estimated in terms of a diffusion coefficient and does not depend on a space grid size.

A PARALLEL ALGORITHM FOR POLYNOMIAL EVALUATION

Ayse Kiper (Middle East Technical University, Turkey)

Horner's algorithm of evaluating a polynomial is studied and formulated as a system of equations $Ax = c$, with a special bidiagonal A . Decoupling algorithm proposed by Kowalik and Kumar for solving bidiagonal systems is simplified and modified by showing that only two stages of three stage algorithm is satisfactory to be used to evaluate polynomials. Some numerical results are presented and discussed. It has been seen that the results are comparable with those of Dorn's.

ROUNDING ERRORS IN ROW-ACTION METHODS FOR SOLVING LINEAR SYSTEMS

Philip A. Knight (University of Strathclyde)

In comparison with direct methods for solving linear systems, the literature concerning the propagation of rounding errors in iterative methods is very limited. Most of the analysis that has been done has centered on splitting methods (Gauss-Seidel, SOR, etc.) and it has been shown that instability can occur when the associated splitting matrix is nonnormal. More recently, attempts have been made to determine the effect of rounding errors on Krylov subspace methods, but despite their widespread use, few classes of matrix are known to be numerically stable for these methods.

After reviewing the current literature we turn our attention to a class of methods that share features of both splitting methods (in that they are stationary) and Krylov methods (in that they make use of orthogonality). This is the class of so-called row-action methods. A row-action method is defined to be an algorithm with the following properties:

- no changes are made to the original matrix;
- no operations are performed on the matrix as a whole;

- in a single iterative step access is required to only one row of the matrix; and the only iterate needed is the immediate predecessor.

Such methods can be used to solve rectangular as well as square systems of equations. Our analysis is centered on one particular algorithm, Kaczmarz's method.

Using two styles of analysis—the first similar to that used for splitting methods, and the second adapted from a method used to study conjugate gradients—we determine conditions on a matrix that ensure row-action methods behave in a stable manner.

GENERALISED SK-SPLINE INTERPOLATION ON COMPACT ABELIAN GROUPS

Alexander Kushpel (Ukraine Academy of Sciences, Ukraine)

The notion of sk-spline is generalised to arbitrary compact Abelian groups. A class of conditionally positive definite kernels on the group is identified, and a subclass corresponding to the generalised sk-spline is used for constructing interpolants, on scattered data, to continuous functions on the group. The special case of d -dimensional torus is considered and convergence rates are proved when the kernel is a product of one dimensional kernels.

CONSTRUCTION OF LATTICE RULES FOR MULTIDIMENSIONAL QUADRATURE

T. N. Langtry (University of Technology, Australia)

Popular methods for approximating multidimensional integrals over the unit cube in s dimensions include products of one-dimensional rules, the number theoretic rules of Korobov (1959) and others, and Monte Carlo integration. Products of rules are suitable only for problems of low dimensionality, while the Monte Carlo method converges only slowly. Number theoretic rules, like the Monte Carlo method, are equal weight rules which generalise the one-dimensional rectangle rule. The latter is known to perform very well for sufficiently smooth periodic integrands over one or more periods, and number theoretic rules are usually chosen with the aim of generalising this behaviour in higher dimensions, thereby providing an advantage over Monte Carlo integration.

In recent years the development of lattice rules, which generalise the number theoretic rules, has allowed significant progress in this direction. Number theoretic rules are rank 1 lattice rules and the product rectangle rule in s dimensions is a rank s lattice rule. Recent theoretical and numerical evidence suggests that certain other types of rank s rules may be competitive with rules of lower rank. In this talk we describe theoretical and numerical evidence that certain rank s lattice rules whose construction is derived from the theory of Diophantine approximation may be competitive with the best published rules of similar orders.

CALCULATION OF GAUSS-KRONROD QUADRATURE RULES

Dirk Laurie (Potchefstroom University for C. H. E., South Africa)

The Golub-Welsch algorithm for computing Gaussian quadrature formulas requires the symmetric tridiagonal Jacobi matrix of recurrence coefficients of the related orthogonal polynomials as input. We define the Kronrod-Jacobi matrix as the symmetric tridiagonal matrix that produces the $(2n + 1)$ -point Kronrod extension of an n -point Gaussian quadrature formula when used as input to the Golub-Welsch algorithm. The first three-quarters of the Kronrod-Jacobi matrix are the same as the corresponding entries of the Jacobi matrix of the $(2n + 1)$ -point Gaussian formula. We show how to find the remaining entries by an algorithm based on modified moments.

RE-STARTING AN ARNOLDI ITERATION

R. B. Lehoucq (Rice University, U.S.A.) & *D. C. Sorensen* (Rice University, U.S.A.).

The Arnoldi iteration is an efficient procedure for approximating a subset of the eigen-system of a large sparse $n \times n$ matrix A . The iteration produces a partial orthogonal factorization of A into an upper Hessenberg matrix H_k of order k . The eigenvalues of this small matrix H_k are used to approximate a subset of the eigenvalues of the large matrix A . The eigenvalues of H_k improve as estimates to those of A as, k , increases. Unfortunately, so does the cost and storage of the factorization.

The idea of re-starting the Arnoldi iteration is motivated by the prohibitive cost associated with building a large factorization. This talk considers two re-starting variants. The first variant, introduced by Saad, *explicitly* re-starts the Arnoldi factorization. The second approach is to *implicitly* re-start the factorization. The implicitly re-started Arnoldi iteration, introduced by Sorensen, is shown to be a truncation of the implicitly shifted QR algorithm.

In exact arithmetic, when using the same starting vector, both algorithms generate the same orthogonal and upper Hessenberg matrices. However, a numerical example is presented that serves to illustrate how both variants may drastically differ in practice. Analysis is presented that explains the generally superior properties of the implicitly re-started Arnoldi iteration.

MODIFIED QUASI-INTERPOLATION ON THE SQUARE USING THIN-PLATE SPLINES

Jeremy Levesley (University of Leicester)

Quasi-interpolation using radial functions is one method of approximation in high dimensions. Typically such approximants are of the form

$$f(x) \approx Q_h f(x) = \sum_{z \in Z^d} f(hz) \psi \left(\frac{x}{h} - z \right),$$

and their analysis involves Fourier transform techniques. In particular, polynomial reproduction depends upon satisfying the Strang-Fix conditions, which are conditions on the Fourier transform on a grid in R^d . However, the normal situation is to have function information only on some compact region of R^d . In this talk we will look at one method of modifying truncated quasi-interpolants in order to recover the full order of approximation observed in the infinite case. We will approximate on a square in two dimensions using thin-plate splines as basis functions.

COMPUTING SPARSE HESSIAN AND JACOBIAN APPROXIMATIONS WITH OPTIMAL HEREDITARY PROPERTIES

Sven Leyffer (University of Dundee) & *Roger Fletcher, Andreas Grothey* (University of Dundee).

In nonlinear optimization it is often important to estimate large sparse Hessian or Jacobian matrices, to be used for example in a trust region method. We propose an algorithm for computing a matrix B with a given sparsity pattern from a bundle of the m most recent difference vectors

$$\Delta = [\delta^{k-m+1} \dots \delta^k], \quad \Gamma = [\gamma^{k-m+1} \dots \gamma^k],$$

where B should approximately map Δ into Γ . In this paper B is chosen such that it satisfies m quasi-Newton conditions $B\Delta = \Gamma$ in the least squares sense.

We show that B can always be computed by solving a positive semi-definite system of equations in the nonzero components of B . We give a necessary and sufficient condition under which this system is positive definite and indicate how B can be computed efficiently using a conjugate gradient method.

In the case of unconstrained optimization we use the technique to determine a Hessian approximation which is used in a trust region method. Some numerical results are presented for a range of unconstrained test problems.

ATTRACTORS AND INERTIAL MANIFOLDS FOR FINITE DIFFERENCE APPROXIMATIONS OF THE COMPLEX GINZBURG-LANDAU EQUATION

G. J. Lord (University of Bristol)

The complex Ginzburg-Landau equation is an example of a dissipative PDE which arises in a large number of scientific fields: from the study of fluid instabilities to superconductivity. As with many other dissipative systems, for the complex Ginzburg-Landau equation there exists an inertial manifold: that is an exponentially attracting, finite dimensional, positively invariant manifold which contains the global attractor.

In this talk we shall consider finite difference approximations to the Ginzburg-Landau equation and consider conditions under which there exists a discrete inertial manifold. To prove existence we make use of a contraction mapping in a Banach space. We then use the contraction property to consider convergence of the approximate and true inertial manifolds.

NORM ESTIMATE FOR INVERSE OF INTERPOLATION MATRIX ASSOCIATED WITH $\|x\|^\alpha$, $1 \leq \alpha < 2$

Zuhua Luo (University of Leicester)

Let $\mathbb{R}^d$ be the d -dimensional Euclidean space. Let $x_1, \dots, x_n$ be n distinct points in $\mathbb{R}^d$ and $\|\cdot\|$ be Euclidean norm on $\mathbb{R}^d$. The radial basis function

$$f(x) = \sum_{j=1}^n a_j \|x - x_j\|^\alpha$$

can be used to interpolate arbitrary data at points $x_1, \dots, x_n$, due to the invertibility of matrix $A = (\|x_i - x_j\|^\alpha)$, $1 \leq \alpha < 2$. In implementing such methods, it is important that A be well conditioned and that its eigenvalues be well bounded away from 0. In this paper, we get lower bounds for the eigenvalues and upper bounds for the inverse of interpolation matrix A . They are all independent of the number of the interpolation points. In the special case of $\alpha = d = 1$, the bounds are sharp.

SOME RECENT WORK IN EXTRAPOLATION QUADRATURE

J. N. Lyness (Argonne National Laboratory, U.S.A.) The earliest application of Richardson's deferred approach to the limit (1923) specifically focussed on numerical quadrature is now known as Romberg Integration (1956). This is based on the Euler-Maclaurin asymptotic expansion for the error functional $E^{(m)}f$ for the m -panel trapezoidal rule approximation $Q^{(m)}f$ to a finite integral If . Romberg Integration is simply one of what is now a wide class of quadrature methods known collectively as Extrapolation Quadrature. A key element in any of these methods is an asymptotic expansion, which resembles the Euler-Maclaurin expansion. In many problem contexts, this expansion is difficult to derive.

By 1985, the theory had been extended to the hypercube and to the simplex, and embraced integrand functions having sophisticated multidimensional algebraic and logarithmic singularities.

During the last ten years, research in this direction has been spurred by the development of finite element methods for boundary value problems. In this talk, I shall describe some recent results. These include extensions to Jacobian free integration over curved surfaces, and to integrands involving the Laplacian operator, and the numerical evaluation of Hadamard finite part integrals has been treated. [This work was supported by the Office of Scientific Computing, U.S. Department of Energy, under Contract W-31-109-Eng-38.]

ANALYSIS AND COMPUTATION OF STEADY OPEN CHANNEL FLOW BY A VANISHING VISCOSITY APPROACH

I. MacDonald (University of Reading) & *M. J. Baines, N.K. Nichols* (University of Reading).

The Saint-Venant equations describe quasi one-dimensional water flow in an open channel and are often used to model the flow in natural rivers. Steady state solutions to these differential equations satisfy a singular nonlinear ODE. We examine this equation along with methods for numerically solving it. In particular we look at the cases where the solution has transitions between subcritical and supercritical which correspond to the solution passing through a singular depth. The method used to study the steady solutions with discontinuities is to regularise the problem by adding a small “viscosity” term to the steady differential equation. The smooth solutions to this regularised equation are examined in the limit of the “viscosity” term vanishing. For a class of useful steady flow problems this approach leads to the existence of a unique physical solution and also to a well-behaved numerical scheme for computing this solution. The scheme is based on the Engquist-Osher scheme.

ADAPTIVE COMPUTATIONS OF THE COMPRESSIBLE EULER EQUATIONS USING A POSTERIORI ERROR ESTIMATES

J. A. Mackenzie (University of Strathclyde)

In this talk we describe the extension of recently obtained *a posteriori* error estimates for finite volume approximations of linear hyperbolic systems to the compressible Euler equations. The error estimates exploit the residual, $\mathbf{r}$, measured in an appropriate weak norm. The derivation of the error estimates is based on the strong stability of an associated linearised dual problem in a manner similar to the *a posteriori* analysis of Johnson and Szepessy. Two-sided estimates of the L_2 norm of the error are then obtained in terms of an adjoint dual graph norm of the finite volume residual. We consider approximations of the adjoint dual graph norm using micro-partitions, and a simpler one-sided residual-based *a posteriori* error bound exploiting $\|h\mathbf{r}\|_{L_2}$, where h is the cell diameter. The main difference between our approach and that of Johnson and Szepessy is that we make no use of Galerkin orthogonality and artificial dissipation. This implies that our estimates are more general in that they are applicable to numerical schemes outside the Galerkin finite element framework, and also to methods which do not introduce artificial dissipation in an explicit fashion.

Obtaining local error estimates is one of the main technical difficulties in the *a posteriori* error analysis of numerical methods for hyperbolic problems. We describe how this can be achieved by splitting the global error into a locally generated component, which we call

the *cell error*, and a non-local component, called the *transported error*, which represents the accumulation of errors generated upwind of a cell and is nearly advected through the cell. It is shown that only the cell error contributes to the cell residual; this justifies our residual-based adaptive strategy for reliable error control.

The *a posteriori* error estimates to be described are similar to those used by Sonar and Süli as local error indicators for the two-dimensional Euler equations of compressible gas dynamics. Calculations of the one-dimensional shock-tube problem will be presented; these demonstrate the sharpness of the error estimates. We will then discuss the implementation of the local error estimates into a simple mesh movement strategy based on equidistributing the finite volume residual.

THE SIMPLEST CLASS OF CYCLING LP PROBLEMS

K. I. M. McKinnon (University of Edinburgh) & *J. A. J. Hall* (University of Edinburgh).

This talk describes a class of linear programming examples which cycle indefinitely and which are the simplest possible examples which show this behaviour. The structure of examples from this class repeat after two iterations. Cycling is shown to occur for both the most negative reduced cost and steepest edge column selection criteria. In addition it is shown that the EXPAND anti-degeneracy procedure of Gill *et al* does not prevent cycling.

THE USE OF THE *W*-METHOD FOR THE NONLINEAR WAVE EQUATIONS

Y. Mai (University of Auckland, New Zealand) & *J. C. Butcher* (University of Auckland, New Zealand).

For many years, the Crank-Nicolson method has been widely used for the time integration in the solution of evolutionary partial differential equations. In this talk, we investigate a higher order method, the *W*-method. This generalises the Rosenbrock method by allowing the Jacobian matrix to be replaced by an arbitrary matrix without lowering its order. A particular four stage third order method of this type is compared numerically with some standard methods using the KdV equation as a test problem. The results for the new method are quite promising. [This work was supported by the FRST Fund, Graduation Research Fund and Mathematics Department Research Fund.]

MIXED INTERPOLATION COLLOCATION METHODS FOR THE NUMERICAL SOLUTION OF VOLTERRA INTEGRAL EQUATIONS WITH PERIODIC SOLUTION

A. Makroglou (University of Portsmouth) *H. Brunner* (Memorial University of Newfoundland, Canada) & *R.K. Miller* (Iowa State University, U.S.A.).

Abstract. We consider the numerical solution of Volterra integral equations with periodic solutions by collocation methods based on the mixed interpolation methods of De Meyer, Vanthournout and Vanden Berghe (1990). The existence and uniqueness of solutions of the problem is examined. Numerical results are given and are compared with these obtained from the application of polynomial collocation methods. A convergence analysis for the exact mixed collocation methods is also included.

A VARIATIONAL APPROACH IN ESTIMATING THE PARAMETER *R* IN INTERPOLATION WITH MULTIQUADRICS

A. Makroglou (University of Portsmouth) & *S.A. Nelson* (Iowa State University, U.S.A.).

A method is presented for the estimation of the parameter *R* in two dimensional multiquadric interpolation. It is based on a variational approach involving an "energy"

functional and it applies also to the case when the function underlying the given data is not known.

A NON-COMPACT FOURTH ORDER NUMERICAL METHOD FOR SOLVING THE STREAM-FUNCTION FORMULATION OF THE NAVIER-STOKES EQUATIONS

Paulo F. de A. Mancera (University of Strathclyde) & *Roland Hunt* (University of Strathclyde).

The Navier-Stokes equations in the streamfunction formulation are solved by a non-compact fourth order numerical method on a non-uniform grid. The accuracy of this numerical method is tested in a channel with gradual constriction. The shape of the channel is determined by a conformal mapping which can give a smooth boundary or one which includes a sharp corner. Results are presented for varying degrees of boundary smoothness and for a range of Reynolds numbers.

A GENERALIZED DISCRETE MULTIPLE SCALES ANALYSIS TECHNIQUE

E. Mare (University of the Orange Free State, South Africa) & *S.W. Schoombie* (University of the Orange Free State, South Africa).

We derive an extension of the discrete multiple scales analysis technique developed by Schoombie [1] We show the similarity between the generalized technique and results obtained by a continuous multiple scales analysis for the Korteweg-de Vries equation.

[1] Schoombie, S.W., *A Discrete Multiple Scales Analysis of a Discrete Version of The Korteweg-de Vries Equation*, J. Comp. Phys. **101** (1992), 55–70.

AUTOMATIC SOLUTION OF FOURTH ORDER SELF-ADJOINT ODE EIGENPROBLEMS

M. Marletta (University of Leicester) & *L. Greenberg* (University of Leicester).

We present a new code, SLEUTH, for numerical solution of fourth order ODE eigenproblems. The code allows the user to obtain an approximation to a specified eigenvalue, rather than to the eigenvalue closest to some initial approximation. Unlike finite difference and variational methods, the cost of computing eigenvalues using SLEUTH does not increase unboundedly as one progresses up the spectrum.

CONVEX DUALITY FOR ESTIMATION PROBLEMS

A.I. Matasov (Moscow Lomonosov State University, Russia) & *V.B. Kolmanovskii* ().

Optimal estimation problems reduce to diverse variational problems. The type and complexity of these variational problems depend on a process model, a model of uncertainties, and an estimation performance criterion. Usually, the variational problems related to estimation are complex and very difficult for numerical solving.

At the same time, mathematical models of real processes are not very accurate as a rule. Therefore, for practical purposes it is often sufficient to find simplified solutions that are not far from the optimal ones. In these cases it is important to evaluate the nonoptimality levels of the approximate solutions *without solving the initial complicated problems*. If the nonoptimality degrees are not large, the considerable expenditure of work needed for computing optimal solutions would not be necessary, and the simplifications would be justified. By means of the duality theory of convex variational problems the estimates for the nonoptimality degrees can be constructed. These estimates can be calculated by relatively simple and numerically effective algorithms.

Our approach is illustrated by two estimation problems. First, a guaranteed estimation problem is considered, when a measurement noise is an unknown but bounded deterministic function. In this case the corresponding variational problem is a nonsmooth one.

Therefore its numerical solving is a nontrivial task. Secondly, a stochastic mean-square filtering problem for dynamic system with delay is investigated. The optimal estimator for this problem requires the solving of functional partial differential equations. So, numerical difficulties are also on hand. For both types of estimation problems simplified numerically effective solving algorithms are proposed. Moreover, the loss in optimality caused by the use of approximate solutions is evaluated.

COMPUTING STABLE MANIFOLDS OF STATIONARY SOLUTIONS

Gerald Moore (Imperial College)

Algorithms for computing stable manifolds for hyperbolic stationary solutions of autonomous systems

$$\dot{\mathbf{u}} = \mathbf{F}(\mathbf{u}) \quad (\dagger)$$

are of two types: either the aim is to compute a single point on the manifold or the entire (local) manifold. Traditionally only *indirect* methods have been considered, i.e. first $(\dagger)$ is discretised by a one-step method and then the Perron-Liapunov or Hadamard graph transform techniques are applied to the resulting discrete dynamical system. We will consider different variants of these indirect methods but also algorithms of the above two types which are applied *directly* to $(\dagger)$.

HIGHER ORDER GODUNOV SCHEMES FOR COMPOSITIONAL MODELLING

A. Morton (University of Reading)

It is often important to incorporate a mathematical description of the oil and the relative proportions of the hydrocarbon components when modelling the flow of oil in underground reservoirs. This detailed compositional breakdown provides a more realistic description of the reservoir fluid—capturing details of the flow of oil and gas that affect gas breakthrough times and oil recoveries. This approach is called Compositional Modelling and is suitable for modelling several important enhanced recovery techniques such as miscible gas injection. The flow equations of this multi-component model are manipulated to form a modified hyperbolic system of conservation laws and a parabolic pressure equation. A review of the flow equations as well as the Higher Order Godunov method, which is used to discretise the hyperbolic part of the system equation, will be given. It is hoped that the techniques used will improve the accuracy of the numerical solution compared to numerical solutions found using standard compositional simulators.

THE DYNAMICS OF A DISCRETISED, NONLINEAR REACTION-DIFFUSION EQUATION WITH DELAY

Tasneem Mukhtar (University of Dundee) & *Desmond J. Higham* (University of Dundee).

We study the long-time behaviour of a discretised evolution equation. The equation, which involves diffusion and a nonlinear, delayed, reaction term, has been proposed as a model in population dynamics. It contains, as special cases, logistic-style problems that have been used before to provide canonical examples of *spurious* behaviour. The existence and stability of true and spurious steady-states are studied, as functions of the grid spacings and problem parameters. Particular attention is paid to the effect of the delay on the long-time behaviour. We also examine the equilibrium states that arise when local error control is used for the time stepping.

PSEUDOSPECTRAL SOLUTION OF NEAR-SINGULAR PROBLEMS USING NUMERICAL COORDINATE TRANSFORMATIONS BASED ON ADAPTIVITY

L.S. Mulholland (University of Strathclyde) *W-Z Huang* (University of Kansas, U.S.A.) & *D.M. Sloan* (University of Strathclyde).

A great deal of attention has been given recently to the use of adaptive grid methods for solving problems with steep fronts/boundary layers. These methods benefit from their ability to cluster meshpoints around and in regions of action; while a non-adaptive grid may require to be very fine throughout the entire domain in order to resolve a localised phenomenon, an adaptive grid will generally require far fewer mesh points to achieve the same resolution. However, great care must be taken when setting up the mesh p.d.e. (to be solved simultaneously with the problem p.d.e.) so that not too many mesh points get thrown into the small region of action.

Rather than attempting to get accurate approximations using an adaptive grid method with many grid points, we use the correspondence between a coarse computational grid and the physical adapted grid to generate a coordinate transformation from physical space to computational space. This transformation maps the original differential equation (with steep-fronted solutions) to a new differential equation with corresponding smooth solutions. Accurate approximations to solutions of the transformed differential equation can then be obtained using a standard Chebyshev-pseudospectral method.

The main difficulty with this approach is in obtaining a coordinate transformation which fits closely the correspondence between points on physical and computational grids and which maintains monotonicity (no grid crossing). Where this difficulty can be overcome, adaptive grid techniques can yield approximations of high-order accuracy, and (pseudo-)spectral methods can retain spectral accuracy on problems with non-smooth solutions.

OPTIMIZATION PROBLEMS IN WAVE ENERGY GENERATION

N.K. Nichols (University of Reading)

Pilot plants for wave energy generation using an oscillating water column (OWC) are now being constructed under the EC Joule II Programme. Strategies for controlling the device to optimize energy extraction over a wide band of the natural sea spectrum are needed. In this paper we will examine three optimization problems arising from the modelling of OWC wave energy devices.

A surface-pressure model of the device response to an incident wave is used, resulting in an integro-differential system equation for the rate of pressure change in the air chamber of the OWC. Different objective functionals for measuring the power generated by the device arise from different models of the losses in the power conversion mechanism. The optimization problem is to maximize the power functional, subject to the system equation. We will examine the theoretical form of the optimal control strategy and discuss numerical methods for solving the optimization problem. Severe difficulties arise for certain choices of the objective function.

A NEW ACCELERATION OF THE PROJECTION METHOD IN NONSYMMETRIC EIGENVALUE PROBLEMS

A. Nishida (University of Tokyo, Japan) & *Y. Oyanagi* (University of Tokyo, Japan).

This study proposes a new method for the acceleration of the projection method to compute a few eigenvalues with the largest real parts of a large nonsymmetric matrix. Saad proposed a Tchebychev acceleration technique for the Arnoldi method, which is an extension of the technique for symmetric matrices. In the nonsymmetric case, we have

to consider the distribution of the eigenvalues in the complex plane. The normalized Tchebychev function $P_n(\lambda) = T_n(\frac{d-\lambda}{c})/T_n(\frac{d}{c})$ has the property

$$\lim_{n \rightarrow \infty} P_n(\lambda) = \begin{cases} 0 & \lambda \text{ is inside of } \hat{F}(d, c) \\ \infty & \lambda \text{ is outside of } \hat{F}(d, c) \end{cases},$$

where d and $d \pm c$ are the center and the focal points of the ellipse $\hat{F}(d, c)$, which passes through the origin. Considering the optimal ellipse which encloses the unnecessary eigenvalues obtained by the previous step of the Arnoldi method and applying this polynomial to the matrix of the problem, we can make the new matrix whose necessary eigenvalues are made dominant. We continue the subsequent Arnoldi iterations with the new matrix. However, the methods based on the optimal ellipse have a defect of making the excessively large ellipse compared with the distribution of the unwanted eigenvalues.

In this paper, we use the convex hull proposed for the solution of the nonsymmetric linear system instead of the Manteuffel's optimal ellipse. The least squares polynomials minimize the L_2 norm defined on the boundary of the convex hull which encloses the unnecessary eigenvalues. From the maximum modulus principle, the absolute value of the polynomial is guaranteed to take on a maximum on the boundary of the convex hull. The polynomials can be generated without any numerical integration, using the orthogonality of the Tchebychev functions. In the eigenvalue problem, we can directly use the orthonormal polynomial generated by the Tchebychev functions as the mini-max polynomial, since we have no need to normalize the polynomial at the origin.

The numerical experiments show that the method is effective for this purpose. Denoting the number of steps of the QR method by n_{QR} and the number of vertices of the convex hull by μ , this method requires the computation of $m_A n^2 + (2m_A^2 + 3m_A - 1)n + 4m_A^2 n_{QR}$ real multiplications and $n_T n^2 + 2n_T n + \frac{1}{2}\mu\{13(n_T)^2 + 31n_T\}$ complex multiplications to obtain the eigenvalues of a matrix of order n , using the Arnoldi method of order m_A and the Tchebychev iteration of order n_T . It is less than those of the method by the Manteuffel's optimal ellipse technique, which requires the solutions of nonlinear equations and $O(n^3)$ computations for every combination of eigenvalues in most cases, and the least squares method, which costs $O(n^3)$ superfluous complexity.

We examined the other problems such as computational error by numerical experiments. Our algorithm shows the best performance in most conditions except for the case where the moduli of some unwanted close eigenvalues is much larger than those of the necessary eigenvalues. We need some additional study for this difficulty.

SPECTRAL PORTRAIT FOR NONHERMITIAN LARGE SPARSE MATRICES

F.Z. Nouri (Universite de Annaba, Algeria)

The spectral portrait of a matrix is the picture of its ϵ -spectra for $\epsilon \in [\epsilon_1, \epsilon_2]$, where an ϵ -spectrum of A is the union of all the eigenvalues of all the matrices $A + \Delta$ with $\|\Delta\|_2 \leq \epsilon\|A\|_2$. The spectral portrait is very useful to study the stability of various problems, for example, we illustrate in this paper to visualise the condition number of an eigenvalue. Some methods to estimate the spectral portrait already exist, but only for small matrices. We propose here a new algorithm to estimate the spectrum for large sparse matrices.

LOCAL, RESTRICTED SPLINES OF DEGREE FIVE

Gerhard Opfer (University of Hamburg, Germany)

We call a spline p *local* if there are only two knots, say $a < b$. The restrictions we have in mind are of the form $c_\ell \leq p \leq c_u$, where c_ℓ, c_u , are given constants. The cases $c_\ell = -\infty, c_u = \infty$ are allowed. A spline p with only two knots is by definition a polynomial. If the polynomial p does not satisfy the given restrictions, a spline x with some additional knots in $]a, b[$ is constructed such that the restrictions are satisfied. An algorithm for constructing non-local splines (i.e. with many knots) can be very efficiently based on the construction of local splines.

For simplicity we treat only non-negativity restrictions, $c_\ell = 0, c_u = \infty$. Mathematically, we treat the variational problem of minimizing

$$f(x) = \int_a^b x'''(t)^2 dt \text{ subject to } x^{(\ell)}(a) = p^{(\ell)}(a), x^{(\ell)}(b) = p^{(\ell)}(b), \ell = 0, 1, 2, x \geq 0.$$

The main discussion is on how many additional knots are needed, how to compute them, and whether there are boundary arcs (meaning that $x = 0$ on a full subinterval). There will be several numerical examples.

A MODEL OF GASFLOW PROBLEM IN 3D BY FINITE ELEMENTS AND SOME APPLICATIONS

Skender Osmani (Polytechnic University, Albania)

We present a study of gasflow problem in a anisotropic heterogeneous media in three dimensional space, resolved by finite element method. The unsteady and steady flow of a real gas is analysed. In addition there are presented some examples of applications in exploitation of Albanian gasfields and well testing.

A PARALLEL SPARSE QR-FACTORIZATION ALGORITHM

Tz. Ostrowski (The Technical University of Denmark) *Per.Christian.Hansen* (The Technical University of Denmark) & *Z. Zlatev* (National Environmental Research Institute, Denmark).

A sparse QR-factorization algorithm for coarse-grain parallel machines will be presented. At the beginning the initial matrix, which is assumed to be general sparse, is reordered properly in an attempt to bring as many zero elements in the lower left corner as possible. Then the matrix is partitioned into blocks of rows and Givens rotations are applied in each of them. These are independent tasks and can be done in parallel. Within a block the rows are processed in proper order in order to exploit efficiently the sparsity of the matrix.

The algorithm can be used for solving least squares problems either independently (as a direct solver) or combined with an appropriate iterative method (for example, Preconditioned CG). In the latter case, dropping of numerically small elements is performed during the factorization stage, which results in better preservation of sparsity and faster factorization, but lack of accuracy in the first solution as well. The iterative method is used to regain the accuracy of the solution in that case.

The numerical results include parallel runs of test examples with matrices from the Harwell-Boeing collection.

TREATMENT OF SPURIOUS SHORT WAVES USING DECOUPLED PETROV-GALERKIN FINITE ELEMENT METHOD

M. Parsaei (Tehran University, Iran) & *R. Wait* (University of Liverpool).

The main obstacle when approximating hyperbolic system of partial differential equations numerically is that an essentially not dispersive media is not replaced by a similar one in the approximation. Consequently, high frequency waves in the numerical model travel with wrong speeds in the wrong directions. An asymptotic analysis of the approximation concentrates on the smooth waves and the problem is not detected. The real physical problems do not possess the smoothness necessary and, in extreme cases, contain shock waves. In such cases it is the mathematical theory of wave motion rather than the asymptotic analysis that determines the behaviour of the waves in the model. Our main concern in this paper is to introduce a new Petrov-Galerkin based approximation method in which the approximating function is assumed to be the superposition of two or more functions, the exact relation between the amplitude of the solution waves at the neighbouring nodes is then determined. It will be shown that in this way the short waves can be decoupled, examined separately and using the Petrov-Galerkin method they can be deformed. The method also increases the number of the free parameters obtainable in the Petrov-Galerkin method which are used to improve the approximation.

To implement the above method we choose the test functions of the Petrov-Galerkin method differently at alternative sets of nodes, as a result the number of difference equations to be analysed are increased. The system of conservation laws $u_t + au_x = 0$ is solved using linear hat functions and the boundaries are assumed to be periodic. Our aim is three fold, first to show that the above method is the right tool to explain the behaviour of the short waves, then to use the method to change the shape of these waves, and finally to increase the order of the approximation using the above free parameters.

ANALYSIS AND SYMBOLIC CONSTRUCTION OF NUMERICAL METHODS FOR $y'' = f(t, y)$

B. Paternoster (Università di Salerno, Italy)

In this talk we explore some possibilities of symbolic computation in the analysis and construction of numerical methods for $y'' = f(t, y)$ using Mathematica [©].

The essence of computer algebra is the possibility to compute expressions leaving the elements of a computation unevaluated. This feature can be used in the construction of numerical method for ODEs, when many properties must be taken into account besides order of consistency, such as dispersive order, stability properties, error constants, and so on.

In particular, we describe a collection of packages to derive Runge–Kutta Nyström (RKN) methods having high dispersive order and good stability properties for ODEs with oscillating solutions. Then we show how an order bound can be obtained through computer algebra for a simple family of composite RKN methods. At last we provide some examples of construction and analysis of new multistep methods, based on trigonometric polynomials, for second order ODEs whose solutions are known to be periodic.

NUMERICAL METHODS FOR COMPUTATION OF MICROSTRUCTURE IN SOLIDS

Petr Plecháč (Heriot-Watt University)

The continuum theory developed by J. Ball and R. James shows a connection between the fine microstructure that is observed in solids under phase transformation, and minimizing sequences of free energy. The variational formulation of the steady-state problem suggests attempting a direct numerical minimization of the discretized energy functional.

However, the energy density is typically represented by a non-convex function and therefore standard minimization methods cannot be used.

We will present two different approaches to overcome this and other difficulties. Numerical solution of a related relaxed problem is very useful, especially for scalar problems, as it allows us to use standard algorithms for minimization problems. The more detailed information about the solution of the relaxed problem helps to control the errors in the approximation and develop an adaptive mesh refinement. Since the vectorial case (which describes general deformation in solids) is essentially more complicated a relaxed problem is not known in an explicit form. Therefore the second method deals with direct minimization on different scales, which produces better approximation of rapid oscillations generated by minimizing sequences. A further postprocessing of the oscillations leads to an approximation of a corresponding Young measure and macroscopic quantities that are measured in physical experiments.

AN ALGORITHM THAT SHIFTS AN ORDERED SEQUENCE OF POINTS ONTO A CURVE M.J.D. Powell (University of Cambridge)

Let $\mathcal{S}$ be any curve in $\mathcal{R}^2$ that is composed of straight line segments and circular arcs, where the pieces are joined so that the direction of $\mathcal{S}$ is continuous, and let $\{\mathbf{p}_j : j = 1, 2, \dots, n\}$ be any finite sequence of points in $\mathcal{R}^2$. We seek a corresponding sequence of points $\{\mathbf{q}_j : j = 1, 2, \dots, n\}$, arranged in order along $\mathcal{S}$, such that the greatest of the Euclidean distances $\{\|\mathbf{p}_j - \mathbf{q}_j\| : j = 1, 2, \dots, n\}$ is as small as possible. We begin by calculating the minimax distance in a way that fixes at least one of the points $\{\mathbf{q}_j : j = 1, 2, \dots, n\}$, and we let $\mathcal{J}$ be the set of indices such that some freedom remains in $\mathbf{q}_j$, $j \in \mathcal{J}$. Then, if $\mathcal{J}$ is not empty, we address the problem of using the freedom to minimize the greatest of the distances $\{\|\mathbf{p}_j - \mathbf{q}_j\| : j \in \mathcal{J}\}$ subject to the original ordering conditions. Thus the initial calculation can fix at least one of the points $\{\mathbf{q}_j : j \in \mathcal{J}\}$, so we work recursively until $\mathcal{J}$ becomes empty. At first sight there are severe difficulties, because fluctuations in $\mathcal{S}$ are liable to induce many local minima in the minimax objective function. We will find, however, that the problem can be solved efficiently. Indeed, the numerical results of a new algorithm show that typically the total work is approximately linear in the sum of n and the number of pieces of $\mathcal{S}$, even if $\mathcal{S}$ crosses itself a hundred times.

NUMERICAL METHODS FOR QUADRATIC ODES

Geetha Ramaswami (University of Cambridge) *Arieh Iserles* (University of Cambridge) & *Mark Sofroniou* (Wolfram Research, U.S.A.).

Many ODE systems of interest share the feature that $\mathbf{y}'$ is a quadratic function of the elements of $\mathbf{y}$. Since some of the elementary differentials in their expansion vanish, there is a considerable reduction in the number of order conditions for Runge-Kutta methods for such systems. We show that this can be exploited to achieve higher order or to minimise the error coefficients.

Some of the separable Hamiltonian ODE's fall under the same category, namely when the Hamiltonian is a multivariate cubic polynomial. We obtain for example six-stage symplectic Runge-Kutta–Nyström methods of order six for such Hamiltonian ODE's. We present numerical experiments on specific examples.

NUMERICAL ANALYSIS OF DIFFERENTIAL-ALGEBRAIC-INTEGRAL EQUATIONS ARISING IN MODELS OF CATALYTIC COMBUSTION

Yuhe Ren (University of Bath) & *A. Spence* (University of Bath).

Coupled systems of differential-algebraic-integral equations (DAIEs) occur in the modelling of catalytic combustion in many chemical engineering situations. These equations have several special features for which there is little or no standard theory. First, the kernel in the integral equation is badly behaved. Second, the coupling of the differential-algebraic equations with the integral equations is completely new and so no software exists to solve such problem. The numerical methods are derived for the types of DAIE which arise in the combustion applications.

ELEMENT RESEQUENCING FOR USE WITH A MULTIPLE FRONT ALGORITHM

Jennifer A. Scott (Rutherford Appleton Laboratory)

The multiple front algorithm is an extension of the frontal method to allow parallelism to be exploited in the solution process. The finite-element domain is partitioned into a number of subdomains and a frontal decomposition is performed on each subdomain separately. For a given partitioning of the domain, the efficiency of the multiple front algorithm depends on the ordering of the elements within each subdomain. We look at the limitations of existing element reordering algorithms when applied to a subdomain and consider how these limitations may be overcome. Extensive numerical experiments are performed on a range of practical problems and, on the basis of the results, we propose a new element resequencing algorithm for use with a multiple front algorithm.

THE APPROXIMATION OF AN EIGENVECTOR BY RITZVECTORS

Paul Smit (Katholieke Universiteit Brabant, The Netherlands)

Eigenvalue algorithms belonging to the class of the Rayleigh-Ritz methods (Krylov-space methods for example) use ‘projections’ on subspaces to produce approximations to eigenvalues and eigenvectors of a matrix. Here we will focus on the eigenvectors. Two angles are important when considering an eigenvector: the angle between the eigenvector and the best approximating Ritzvector and the angle between the eigenvector and the subspace involved. It is studied how an upperbound for the first angle can be expressed in terms of the second one. This results in a theoretical expression for the case of two-dimensional subspaces and a conjecture for higher dimensional subspaces supported by numerical experiments.

SEMI-LAGRANGIAN METHODS IN NUMERICAL WEATHER PREDICTION

C.J. Smith (University of Reading) & *M.J. Baines* (University of Reading).

Recent years have seen the rapid development of the semi-Lagrangian method, for the treatment of advection in numerical weather prediction. This method offers an advantage in computational speed over Eulerian methods of discretisation. This is achieved by allowing accuracy considerations alone to dictate the length of the time step. However, this must be balanced by the loss of existing theory supporting Eulerian methods. Loss of strict conservation of advected quantities raises particular concern in many applications. Further problems arise, where important phenomena propagate with other than the velocity of the flow. Generation of standing waves near mountains provides one example. We shall describe the semi-Lagrangian method and briefly review some aspects of current implementations.

ANALYSIS OF EQUIDISTRIBUTION-BASED MOVING MESH SCHEMES FOR 1-D DISSIPATIVE PARTIAL DIFFERENTIAL EQUATIONS

Jeremy H. Smith (Stanford University)

Like most numerical methods, moving meshes are discretizations of a continuous principle. We begin by analyzing a continuous framework for equidistribution-based moving mesh schemes. Analysis in this framework provides a model for analysis of the semi-discrete equations. We prove several properties of moving mesh schemes that are inherited from the continuous framework, and prove convergence in the Lax-Richtmeyer sense of the semi-discrete equations for a certain class of PDEs. Numerical examples will be given demonstrating the computational efficiency of moving mesh methods.

NUMERICAL SOLUTION OF THE BECKER-DÖRING EQUATION

A. R. Soheili (Heriot-Watt University)

The Becker-Döring equations are an infinite system of ordinary differential equations describing coagulation and fragmentation of clusters of identical particles. Clusters coagulate by gaining or fragment by losing single particles. The Becker-Döring equations are usually approximated by a truncated finite dimensional system of ordinary differential equations, but this can still be very large.

Here a reduced model of this system is discussed, where clusters are treated together in a small groups, and a simple behaviour is assumed within each group. There is a very close agreement between the results of this model and the full model. The numerical solution of the full model was studied by Carr, Duncan and Walshaw in 1993.

FACTORIZING A RATIONAL FUNCTION FROM ITS VALUES AT THE ROOTS OF UNITY

P. G. Spain (University of Glasgow)

Let ϕ be a rational function with r poles, let N be an integer, and suppose we are given, as sample-values, the values of ϕ at the N^{th} roots of unity. We use the values of the Discrete Fourier Transform to construct a finite Hankel matrix Φ . The condition $N \geq 2(r + 1)$ ensures that Φ_r is invertible while Φ_{r+1} has rank r and nullity 1 : here Φ_s is the top-left $s \times s$ corner of Φ .

If $(\alpha_1, \dots, \alpha_r)$ are the poles of ϕ , and P is the column vector of coefficients of the polynomial whose roots are $(\alpha_1, \dots, \alpha_r)$, then

$$\Phi_{r+1} P = 0.$$

This is the crucial relationship which allows us recover $(\alpha_1, \dots, \alpha_r)$ from Φ , so long as we can detect the value of r . We show how to find r by exploiting this relationship both for ϕ and its reciprocal.

DETERMINISTIC AND PROBABILISTIC ANALYSIS OF ADAPTIVE ALGORITHMS FOR INITIAL-VALUE PROBLEMS

Andrew Stuart (Stanford University, U.S.A.)

The numerical solution of initial value problems for ordinary differential equations is frequently performed by means of adaptive algorithms with user-input tolerance τ . The time-step is then chosen according to an estimate, based on small time-step heuristics, designed to ensure that the local error committed per unit step is proportional to τ . A question of natural interest is to determine how the global error behaves with respect to the tolerance τ . This has obvious practical interest and is also a challenging problem in mathematical analysis. The primary difficulties arising in the analysis are that: (i)

the time-step selection mechanisms used in practice are discontinuous as functions of the specified data; (ii) the small time-step heuristics underlying the control of the local error can break down in some cases.

In this talk an analysis is presented which incorporates these two difficulties. The breakdown of the small time-step heuristics can be incorporated in the analysis by making minor modifications to standard algorithms used in practice, leading to a deterministic convergence proof for the global error of such algorithms as $\tau \rightarrow 0$. Alternatively, it may be shown that in a certain probabilistic sense, with respect to a measure on the space of initial data, the heuristics are valid with probability one, leading to a probabilistic convergence result for the global error as $\tau \rightarrow 0$.

ESTIMATING THE ACCURACY OF CERTAIN ENGINEERING APPROXIMATIONS FOR CONFORMAL MODULES OF QUADRILATERALS

N. Stylianopoulos (University of Cyprus) & *N. Papamichael* (University of Cyprus).

The conformal module $m(Q)$ of a quadrilateral $Q := \{\Omega; z_1, z_2, z_3, z_4\}$, consisting of a Jordan domain Ω and four points z_1, z_2, z_3, z_4 , in counterclockwise order on $\partial\Omega$ is defined as follows: Let R_H denote a rectangle of base 1 and height H of the form $R_H := \{(x, y) : 0 < x < 1, 0 < y < H\}$. Then, $m(Q)$ is the unique value of H for which Q is conformally equivalent to the rectangular quadrilateral $\{R_H; 0, 1, 1+iH, iH\}$. That is for $H = m(Q)$ and for this value only there exists a unique conformal map $\Omega \rightarrow R_H$ which takes the four points z_1, z_2, z_3, z_4 , respectively onto the four corners $0, 1, 1+iH, iH$ of R_H .

In this talk we consider certain engineering rules for approximating the conformal modules of quadrilaterals, due to P.M. Hall [Thin Solid Films **1** (1967/68), 277-295]. By making use of the theory of a domain decomposition method for conformal mapping (N. Papamichael and N.S. Stylianopoulos [Numer. Math. **62** (1992), 213-234]) and, in particular, of certain results for a special class of quadrilaterals, due to D. Gaier and W. Hayman [Constr. Approx. **7** (1991), 453-467], we derive error estimates for the above rules. These estimates show that the rules are, in fact, remarkably accurate.

FINITE ELEMENT METHODS FOR CONVECTION-DIFFUSION PROBLEMS USING EXPONENTIAL SPLINES ON TRIANGLES

Martin Stynes (University College, Republic of Ireland) & *Riccardo Sacco* (Politecnico di Milano, Italy).

We consider linear singularly perturbed elliptic problems (such as linearised convection-dominated flow problems) in two dimensions. The solutions to such problems typically exhibit boundary and interior layers and are difficult to solve numerically. To compute numerical solutions, we use a new family of Petrov-Galerkin finite element methods on triangular grids. Our method incorporates divergence-free trial functions that form a natural generalization of one-dimensional exponential trial functions. The family includes an improved version of the divergence-free finite element method used in the PLTMG code. Numerical results show that the new method is able to compute strikingly accurate solutions on coarse meshes.

COMPUTING METHOD PARAMETERS FOR PARALLEL IMPLICIT RUNGE-KUTTA METHODS

Jacques J.B. de Swart (CWI, The Netherlands)

Among the most powerful methods for numerically solving ordinary differential equations

is the family of implicit Runge-Kutta methods. However, these methods require a lot of computational effort on a sequential computer. By substituting a matrix B for the Runge-Kutta matrix A , it is possible to make the method suitable for parallel implementation. In this talk we address the problem of finding matrices B that offer the possibility of parallelization, but still resemble A . By using the special structure of Runge-Kutta matrices, it is, under certain conditions, possible to prove the existence of a special choice for B .

MODELLING FLOW IN GAS PIPELINES

J. D. Taylor (Heriot-Watt University)

British Gas operates a large pipeline network in the UK, transmitting natural gas from coastal terminals to the local networks for distribution to the user. Gas flow in the transmission network typically changes rather slowly, and can usually be simulated using a simplified quasi-steady approximation which takes big time steps and is computationally inexpensive. However, in regions undergoing rapid change the full gas dynamics equations must be used, and the computational effort is then much greater. The cost of using the full gas dynamic model throughout the network is prohibitive. We discuss methods to split the network into fast and slow changing areas where the different models of gas flow are solved by numerical methods using different time step sizes. The problem to be addressed is how to interface the different regions.

BOUNDARY ELEMENT METHOD SOLUTION OF TRANSIENT HEAT CONDUCTION PROBLEM

Münevver Tezer-Sezgin (Middle East Technical University, Turkey)

A boundary element method (BEM) formulation is presented to obtain the solution of the transient heat conduction problem. The time derivative in the equation is approximated by the time-stepping scheme, thus, the problem is formulated in the form of an in homogeneous modified Helmholtz equation. The BEM with linear elements is 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 unknown boundary values only. The solution of this integral equation presents none of the problems encountered in interior methods. The difficulty arising from the domain integral due to the source function is eliminated by obtaining an approximate particular solution to the equation. This is done by a very simple procedure approximating both the source function and the particular solution as a linear combination of several radial basis functions simultaneously.

HIGH ORDER, P-STABLE METHODS FOR SECOND ORDER INITIAL VALUE PROBLEMS IN ORDINARY DIFFERENTIAL EQUATIONS

R. M. Thomas (UMIST)

We consider a family of implicit two-step methods for solving nonlinear initial value problems

$$\ddot{y} = f(t, y), \quad y(0), \quad \dot{y}(0) \text{ given.}$$

By evaluating the differential system at a number of additional off-step points, P-stable methods of order up to eight can be derived. The remaining free parameters of the methods can be chosen, for example, to reduce the amount of computational effort required when using the methods. We discuss also a technique for estimating the local error in these methods.

OPTIMAL MESHES FOR L_2 APPROXIMATION BY DISCONTINUOUS PIECEWISE POLYNOMIALS

Y. Tourigny (University of Bristol) & *M. J. Baines* (University of Reading).

We shall discuss the problem of constructing an optimal mesh for the best L_2 approximation of a given function by discontinuous piecewise polynomials. In the one-dimensional case, it can be shown that, under certain assumptions concerning the function to approximate, Baines' algorithm [M.J. Baines, *Math. Comp.*, 62 (1994), pp. 645-669] for piecewise linear or piecewise constant polynomials with self-adjusting nodes produces a mesh sequence which converges to an optimal mesh. In two dimensions, a modification of this algorithm is combined with Lawson's LOP algorithm. Optimal triangulations of the unit square will be shown for a range of interesting test functions.

APPROXIMATING PSEUDOSPECTRA BY THE ARNOLDI ITERATION

Lloyd N. Trefethen (Cornell University, U.S.A.) & *Kim-chuan Toh* (Cornell University, U.S.A.).

The Arnoldi iteration, usually viewed as a method for calculating eigenvalues, can also be used to estimate pseudospectra. We present numerical examples and discuss their potential significance.

THE EFFECTS OF PRECONDITIONING ITERATIVE METHODS IN COUPLED DISCRETIZATION OF FLUID FLOW PROBLEMS

Paulo B. Vasconcelos (Universidade do Porto, Portugal) & *Filomena D. d'Almeida* (Universidade do Porto, Portugal).

The progress achieved in parallel computer architectures allows for the treatment of larger and larger problems. Computational Fluid Dynamics, where simulations require large computation times, is one of the areas of application of high performance computing. Schemes such as the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm are often used to solve the discrete Navier-Stokes equations. Generally and for simpler domain geometries these schemes are fast to converge but require a large number of iterations. However, the decoupling of the differential equations involved implies a slow convergence of rotationally dominated problems and can be very time consuming for realistic applications. With recent advances in hardware technology and software design, it became possible to solve coupled Navier-Stokes systems, which are more robust but imply increasing computational requirements (both in memory and CPU time). We will describe two approaches (band block LU factorization and preconditioned GMRES) for the linear solver required by the DIRECTO algorithm that solves the fluid flow equations as a coupled system. We will compare the effectiveness of incomplete factorization preconditioners applied to GMRES (Generalized Minimum RESidual) method and present some numerical results showing that it is possible to greatly minimize the CPU time of the coupled approach and that there are cases where it can be faster than the decoupled one. [We would like to thank Prof. Ian Duff and CERFACS for the invitation to stay at CERFACS in July 1994.]

STEP-PARALLEL RUNGE-KUTTA METHODS

W.A. van der Veen (Centre for Mathematics and Computer Science, The Netherlands)

A well known class of methods for solving stiff ODEs is the class of Implicit Runge-Kutta (IRK) methods. From a theoretical point of view IRKs are ideal methods since they can combine an arbitrarily high order with unconditional stability. In practice, however,

these methods have the disadvantage that they are very expensive. One way to reduce the costs is by applying parallelism. Recently several of such methods have been developed at CWI. These methods solve the IRK equation by a parallel, diagonal iteration process and are called PDIRK methods. It turned out that high-order PDIRK methods are more efficient than the corresponding IRKs.

A drawback of high-order PDIRK methods is that they require quite a large number of iterations. To circumvent this, we developed step-parallel methods based on the PDIRK method. In these new methods, the *effective* number of iterations is much lower. The step-parallel methods start iterating in the next point on the t-axis as soon as the iterate in the current point is sufficiently accurate. In this way, iteration processes in several points on the t-axis are performed simultaneously. Determining whether a point is sufficiently accurate is done by means of a carefully designed strategy. We have succeeded in formulating a strategy that is both efficient and robust. Experiments show that the speedup with respect to PDIRK ranges from 2 to 3.

COMPARISON OF PARALLEL COMPUTERS USING AIR POLLUTION MODELS

Jerzy Wasniewski (The Technical University of Denmark)

To compare the performance and use of parallel computers, we implemented a large air pollution model on several computer platforms. Using a realistic large-scale model, we have gained detailed insight about the performance of these computers to solve large-scale scientific problems that involve several types of numerical computations. The computers involved in our study are the Connection Machines CM-200 and CM-5, the MasPar MP-2216, KSR1, Cray T3D, Convex SPP, IBM-SP2, SGI Power Challenge and a cluster of workstations using the PVM system.

THE CONVERGENCE RATE OF FINITE ELEMENT APPROXIMATIONS ON EQUIDISTRIBUTED GRIDS

Andy Wathen (University of Bristol) & *Paul Selwood* (University of Leeds).

The use of irregular gridding for numerical solution methods for ordinary and partial differential equation boundary value problems is widespread. In particular this is true of the geometrically flexible finite element method. Convergence rates, however, are usually expressed in terms of ‘the maximal mesh size’ h and most often do not account for the irregularity of local mesh sizes. Error estimates in terms of h have the usual asymptotic meaning in Numerical Analysis expressing the rate at which the error should reduce as $h \rightarrow 0$. Such estimates are descriptive of the error on any particular grid in so far as this rate would be observed under any quasi-uniform refinement.

In this talk we consider irregular grids in the context of refinement paths, i.e. sequences of grids such that $h \rightarrow 0$. In particular, we will consider grids generated from common ‘equidistribution’ principles which do not give rise to quasi-uniform meshes even for simple problems. The rate of convergence of piecewise polynomial approximations on such meshes is then not described by the usual theory.

We will present a result relating the ‘monitor’ function which is equidistributed to the ‘mesh function’ which describes the refinement path. We will go on to show that unusual asymptotic convergence rates in the sense of $h \rightarrow 0$ are obtained even with very practical choices of monitor function. Asymptotic descriptions of errors in terms of ‘mesh functions’ and the number of degrees of freedom in an approximation are also possible and we will discuss conditions under which the different descriptions are equivalent, and conditions under which they can be (markedly) different.

Time permitting, numerical results for a particular refinement in two space dimensions will be given which demonstrate that these observations of unusual convergence behaviour on irregular grids are not just a one-dimensional feature.

USE OF THE HUBER M-ESTIMATOR FOR THE ERRORS-IN-VARIABLES PROBLEM

G. A. Watson (University of Dundee) & *D. Hermey* (University of Dundee).

Various techniques are now available for solving data fitting problems where there are errors in all variables, e.g. total least squares, orthogonal distance regression etc. Here the use of the Huber M-estimator is considered in this context.

COMPUTING THE HILBERT TRANSFORM ON THE REAL LINE

Andre Weideman (Oregon State University, U.S.A.)

We present a method for computing the Hilbert integral transform, defined by

$$\mathcal{H}\{f\}(y) = \frac{1}{\pi} \text{PV} \int_{-\infty}^{\infty} \frac{f(x)}{x-y} dx.$$

It is a collocation method, based on an expansion in rational eigenfunctions of the Hilbert transform operator. It can be implemented through the Fast Fourier Transform. Error formulas and convergence rates for some simple classes of functions will be discussed. Comparisons with other methods will be presented, as well as an application of the method to the Benjamin-Ono equation, defined by

$$u_t + uu_x + \mathcal{H}\{u_{xx}\} = 0.$$

ON ASYMPTOTIC ERROR EXPANSIONS FOR SINGULAR BOUNDARY VALUE PROBLEMS

Ewa B. Weinmüller (University of Technology, Austria) & *Florian Frommlet* (University of Technology, Austria).

In this paper we discuss the existence of an asymptotic expansion for the global error of a simple finite difference method when applied to solve boundary value problems for ordinary differential equations with a singularity of the first kind. During the last years there has been a considerable progress in the theory of approximations to solutions of singular problems. For wide classes of methods (finite differences, collocation methods, multistep-methods) stability results and global error bounds have been derived.

An effective technique for the numerical solution of ODEs is the *Iterated Defect Correction Method*, IDeC, originally proposed as a method for the estimation of the global error. We use IDeC to solve the problem

$$y''(t) = f\left(t, \frac{y(t)}{t^2}, \frac{y'(t)}{t}\right), \quad 0 \leq t \leq 1, \quad y(0) = \alpha, \quad y(1) = \beta,$$

with the exact solution $z(t)$. The first, basic approximation $\zeta^{(1)}$ for z , is obtained from the standard three-point finite difference scheme realized on an equidistant grid with stepsize h . In the course of the IDeC iteration this solution is gradually improved and the iteration terminates after the required accuracy has been reached.

It is an important goal to quantify the accuracy of the computed sequence of approximations $\zeta^{(i)}$, by deriving error bounds of the form

$$\|\zeta_\nu^{(i)} - z(t_\nu)\| \leq c \cdot h^{p_i},$$

which hold for all gridpoints t_ν . For “classical” problems, $f = f(t, y(t), y'(t))$, with smooth data one can show (under appropriate assumptions on the iteration) that $p_i = 2i$, $i \geq 1$, holds up to a certain upper bound (depending on technical features of the IDeC procedure). Obviously, the constant c may depend on the problem’s data but not on h , and it can be shown that it is moderately sized for all t_ν .

Here we investigate the structure of the global discretization error for certain classes of *singular* problems. We discuss typical situations and explain how the features of the problem and its solution z influence the form of the asymptotic error expansions and their final length. We also show under which circumstances full asymptotic expansion exist. To illustrate the theory we present experimental results from the IDeC computations.

CONVERGENCE OF CHORIN’S ORIGINAL PROJECTION SCHEME

Brian R. Wetton (University of British Columbia, Canada)

Chorin’s original projection scheme for the incompressible Navier-Stokes equations from 1968 is considered. The spatial discretization is formally second order in space size h and the time discretization is first order in time step k with the projection part of the Stokes operator split off for computational efficiency. If it is assumed that $k = \lambda h^2$ convergence of first order in k might be expected. While this is true for the velocity, it is not true for the pressure. In fact, the discrete pressure from Chorin’s method has an $O(k^{1/2})$ numerical boundary layer due to the projection step and an $O(h)$ global error due to an amplification of checkerboard modes in the velocity. The error analysis of the projection step follows the work of E and Liu and the analysis of the checkerboard modes is due to the author. The two are combined to show the asymptotic character of the errors in the scheme. Convergence is shown using discrete energy estimates.

THE USE OF GAUSSIAN COLLOCATION FOR ORDINARY DIFFERENTIAL INITIAL VALUE PROBLEMS WITH SINGULAR POINTS

K. Wright (University of Newcastle upon Tyne)

It is well known that collocation using Gauss points has important properties relating to stability and accuracy. There are also rather special properties of the method when used to solve initial value problems with singular points.

It will be shown that for suitable test problems the collocation matrix will be singular in clearly defined circumstances. In fact, this will happen if the singular point is at the upper end of the interval or at a zero of an orthogonal polynomial related to the corresponding Legendre polynomial (though not the Legendre polynomial itself).

It will also be shown that for these test problems exact results will be obtained at the end points of intervals even when the true solution has a simple pole inside one of the intervals of integration.

The relevance of these results for the numerical solution of equations with singular points will be considered.

POINT-BASED SET-VALUED APPROXIMATION AND NEWTON’S METHOD

Huifu Xu (Ningbo University, P. R. China, presently Visiting Scholar, University of Dundee)

In this paper, a kind of point-based set-valued approximation (PBSVA) is introduced for general locally Lipschitz continuous vector-valued functions. It is found that the set-valued mappings involved in a PBSVA can be defined by the support bifunctions based on the Clarke’s generalized derivatives, the upper Dini directional derivatives and the Michel-

Penot generalized directional derivatives. Consequently, a unified framework of Newton's method for nonsmooth equations is established, and it is proved that whether they are locally superlinearly convergent to a solution depends on to a large extent whether the functions involved admit a nonsingular PBSVA in the neighborhood of the solution point. Finally, cases are studied, by which, some new generalized Newton methods based on the Dini generalized Jacobian and the Michel-Penot generalized Jacobian are derived, and some present Newton-like methods are explained from a unified viewpoint.

WEIGHTED QUADRATURE IN KRYLOV METHODS

R.V.M. Zahar (Université de Montréal, Canada) *J.D. Lawson* (Algoma University College, Canada) & *S.J. Thomas* (Recherche en prévision numérique, Dorval, Canada).

The Krylov subspace approximation techniques introduced by Gallopoulos and Saad for the numerical solution of parabolic partial differential equations are extended. By combining the weighted quadrature methods of Lawson and Swayne with the Krylov subspace algorithm, three major improvements are made. First, problems with time-dependent sources or boundary conditions may be solved more efficiently. Second, methods are derived which have the stability properties (such as A-stability) of the underlying rational approximation to the exponential function. Third, it is possible to formulate procedures which are robust under space discretization refinement. In particular, a fixed precision is maintained for the same time integration method and for constant values of the parameters, when the spatial resolution is increased.

NUMERICAL ANALYSIS OF TODA FLOWS

Antonella Zanna (University of Cambridge) *Maripaz Calvo* (Universidad de Valladolid, Spain) & *Arieh Iserles* (University of Cambridge).

Toda lattice equations arise in a wide range of applications, e.g. quantum mechanics and soliton dynamics. Moreover, well known numerical algorithms, like the QR method for finding eigenvalues, can be formulated as a flow on a Toda lattice. The most important qualitative feature of the flow is its *isospectrality*. However, when classical numerical ODE methods are applied to solve the problem, isospectrality is usually lost. Instead we propose a different approach, based on the Lax formulation of the Toda lattice equations and their theoretical analysis by Flaschka. This generalizes the RK approach, thereby leading to isospectral methods of arbitrarily high order for the underlying problem.

List of Participants

Invited Speakers

J C Butcher	University of Auckland
G H Golub	Stanford University
A Griewank	Technical University of Dresden
D F Griffiths	University of Dundee
R Jeltsch	ETH Zurich
W Light	University of Leicester
K W Morton	University of Oxford
B N Parlett	University of California Berkeley
L Petzold	University of Minnesota
R D Russell	Simon Fraser University
J M Sanz-Serna	Universidad de Valladolid
D J Silvester	UMIST
E Suli	University of Oxford
M H Wright	AT & T Bell Laboratories
J Zowe	University of Bayreuth

Algeria

M L Hadji	University of Annaba
F Z Nouri	University of Annaba

Albania

S Osmani	University of Tirana
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Australia

K Burrage	University of Queensland
J A Belward	University of Queensland
T N Langtry	University of Technology, Sydney

Austria

E Weinmueller	Technische Universitaet Wien
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Belgium

G Vanden Berghe	University of Gent
M Van Daele	University of Gent

Canada

H Brunner	Memorial University
X Chang	McGill University
T F Fairgrieve	University of Toronto
P Keast	Dalhousie University
B Wetton	University of British Columbia
R Zahar	Université de Montréal

China

H Xu	Ningbo University
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Cyprus

N Stylianopoulos

University of Cyprus

Denmark

T T Ostromsky

Technical University of Denmark

J Wasniewski

The Danish Computer Centre

France

P Chartier

IRISA

G Decamps

ENSEEIH

J Y l'Excellent

ENSEEIH

O Marques

CERFACS

E Noulard

ENSEEIH

Germany

E Buckwar

Freie Universitat Berlin

G Opfer

University of Hamburg

Honk Kong

J Caldwell

City Polytechnic of Hong Kong

Iran

M Parsaei

Tehran University

Ireland

M Stynes

University College Cork

Israel

A Dax

Hydrological Service

Italy

M Arioli

IAN-CNR

L Lopez

University of Bari

A Paone

National Research Council - Naples

B Paternoster

Universita di Salerno

A Vecchio

National Research Council - Naples

M I C Vieira

Japan

A Nishida

University of Tokyo

Lithuania

R Čiegis

Inst for Mathematics and Informatics

The Netherlands

K Dekker

Delft University of Technology

P J van der Houwen

CWI, Amsterdam

P Smit

Katholieke Universiteit Brabant

J de Swart

CWI, Amsterdam

W van der Veen

CWI, Amsterdam

New Zealand

Mai Ying
University of Auckland

Norway

R P K Chan
T Havie
The Norwegian Institute of Technology
University of Trondheim

Portugal

T Diogo
F G Martins
P B de Vasconcelos
Instituto Superior Tecnico
Universidade Nova de Lisboa
Universidade do Porto

Russia

A I Matasov
Moscow Lomonosov State University

South Africa

D P Laurie
E Mare
Potchefstroom University
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Spain

B Garcia-Archilla
C Gonzalez
Universidad Autonoma de Madrid
Universidad de Valladolid

Switzerland

J P Berrut
M D Buhmann
Universite de Fribourg
ETH

Sweden

Å. Björck
M Reifenberg
Linköping University
Universite de Fribourg

Turkey

A Kiper
M Tezer-Sezgin
Middle East Technical University
Middle East Technical University

United Arab Emirates

M Al-Baali
UAE University

UK

M Ainsworth
I Al-Subeyhi
A H Alim
R Astley
M Aves
M J Baines
C T H Baker
K E Barrett
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G Burnside	University of Dundee
F F Campos	University of Oxford
Z A Cinar	Brunel University
J P Coleman	University of Durham
G Collins	Bristol University
B Davidson	Aspentech UK Ltd
F Davidson	University of Dundee
P J Davies	University of Dundee
C Dixon	University of Dundee
M Drexler	Oxford University
I S Duff	Rutherford Appleton Laboratory
D B Duncan	Heriot Watt University
K J Edwards	University of Dundee
G A Evans	De Montford University
R Ferguson	University of Bath
S Fleming	University of Dundee
R Fletcher	University of Dundee
N Ford	Chester College
T L Freeman	University of Manchester
T N T Goodman	University of Dundee
G Goodsell	University of Cambridge
N I M Gould	Rutherford Appleton Laboratory
P R Graves-Morris	University of Bradford
A K Griffith	University of Reading
A Grothey	University of Dundee
J A J Hall	University of Edinburgh
D C Handscomb	University of Oxford
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N J Higham	University of Manchester
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P Houston	University of Oxford
A R Humphries	University of Bristol
R Hunt	University of Strathclyde
A Iserles	University of Cambridge
R J Jarvis	University of Dundee
T Johnson	University of Dundee
D S Jones	University of Dundee
T Kelsey	University of Dundee
S Keras	University of Cambridge
P Knight	Strathclyde University
A Kushpel	Kiev University
C Lamb	University of Dundee

A Lambert	University of Dundee
J Levesley	University of Leicester
S Leyffer	University of Dundee
Y Liu	University of Cambridge
G Lord	University of Bristol
Zuhua Luo	University of Leicester
I MacDonald	University of Reading
J A Mackenzie	University of Strathclyde
A Makroglou	University of Portsmouth
P F de A Mancera	University of Strathclyde
C Maple	University of Leicester
M Marletta	University of Leicester
G Mathai	University of Dundee
M McCallum	Strathclyde University
K McKinnon	University of Edinburgh
R Middleton	University of Dundee
A R Mitchell	University of Dundee
G Moore	Imperial College
A Morton	University of Reading
T Mukhtar	University of Dundee
L Mulholland	University of Strathclyde
M Murphy	University of Bristol
B Murray	MTD Ltd
N K Nichols	Reading University
V Pennington	NAG Ltd
F Plab	University of Edinburgh
P Plecháč	Heriot-Watt University
M J D Powell	University of Cambridge
Y Q Qiu	Strathclyde University
A Ramage	University of Strathclyde
G Ramaswami	University of Cambridge
Y Ren	University of Bath
D E Roberts	Napier University
G Roussos	UMIST
D Roxburgh	Dundee University
B Russell	University of Dundee
J Scott	Rutherford Appleton Laboratory
B D Sleeman	University of Dundee
D M Sloan	University of Strathclyde
C Smith	University of Reading
A Soheili	Heriot Watt University
P Spain	University of Glasgow
J Taylor	Heriot Watt University
R Thatcher	UMIST
D P Thomas	University of Dundee
R M Thomas	UMIST
Y Tourigny	University of Bristol

D Tse
R Wain
A J Wathen
G A Watson
L A Wazzan
K Wright
C Yiu
E Young
A Zanna
C Zoppke

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