

18th Dundee Numerical Analysis Conference

June 29-July 2, 1999

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Invited Speakers

The special invited lecture in honour of A. R. Mitchell will be presented by

Professor Franco Brezzi
Università degli Studi di Pavia

The other Principal Speakers who have accepted our invitation are:

Mark Ainsworth	University of Leicester, UK
Françoise Chaitin-Chatelin	CERFACS, France
Tony F. Chan	UCLA, USA
Charles M. Elliott	University of Sussex, UK
Michael C. Ferris	University of Wisconsin, USA
Randall J. LeVeque	University of Washington, USA
Christian Lubich	Universität Tübingen, Germany
Michael J. D. Powell	University of Cambridge, UK
Rolf Rannacher	Universität Heidelberg, Germany
Ian H. Sloan	University of New South Wales, Australia
Paul M. Van Dooren	Université Catholique de Louvain, Belgium
G. Alistair Watson	University of Dundee, UK
Olof B. Widlund	New York University, USA

The after dinner speaker will be Professor David M. Sloan of Strathclyde University.

Abstracts of Invited Talks

A posteriori error analysis of finite element approximations

Mark Ainsworth

Strathclyde University

A priori error estimates have been a staple ingredient of finite element analysis from the outset, but a posteriori error estimates have really only blossomed over the past decade to take their natural place alongside a priori estimates. There are many reasons behind the current explosion of interest in a posteriori error estimates. For instance, such estimators lie at the very heart of an adaptive solution algorithm. In many cases, a posteriori error estimators provide quantitative estimates for the actual error (as opposed to estimates

for the rate of convergence) and, as such, have been fully embraced by many finite element practitioners who have traditionally had little patience for the mathematical niceties of a priori error estimates. The talk will survey some of the main developments in a posteriori error analysis over the past decade.

Interacting with the subgrid world

Franco Brezzi

Università di Pavia

Subgrid phenomena should, by definition, be invisible within the given computational grid, that we might imagine to be the finest grid we can afford to solve a given problem. However, in recent times, attempts have been made to simulate the interactions between the subgrid world and the computational grid. The idea behind these attempts is that we might be satisfied by simulating the effects of such interactions on the computational grid.

Several areas of modern Numerical Analysis can be interpreted in this framework, including homogenisation, LES, and various stabilising techniques that have been developed in different contexts.

There is an effort, taking place in part of the Scientific Computing community, to bring all these procedures and techniques to some common philosophy first, and then to a common mathematical framework.

The talk will describe the most recent successes and failures in this direction, and briefly discuss the possible future perspectives.

Variational PDE Models and Methods for Image Processing

Tony F Chan

University of California at Los Angeles

Variational PDE methods have emerged recently as alternatives to traditional statistical and fast transform based methodologies in image processing. Examples are the Perona-Malik anisotropic diffusion model, the total variation restoration method by Rudin, Osher and Fatemi, the axiomatic derived fundamental PDE due to Alvarez, Guichard, Lions and Morel, the Mumford-Shah segmentation model, and various active contour models for object detection. These PDE models offer a systematic way to treat geometric properties of images, as well as to properly handle singularities (e.g. edges). Through these models, the vast arsenal of PDE and CFD techniques can be brought to bear on image processing problems. On the other hand, these models are usually highly nonlinear and require new computational techniques for their effective solution, including optimization and linearization techniques, as well as level set methods for tracking interfaces.

In my talk, I'll give a brief introduction to this field after which I will highlight some work in our group on the development of efficient numerical methods, as well as new models for multi-spectral and color images, blind deconvolution, active contours, denoising of vector fields, etc.

Nonlinear least squares optimization for precise orbit detection in Spatial Technology. A study of the convergence of Gauss-Newton

F. Chaitin-Chatelin¹ & S. Gratton

¹Université Toulouse I et CERFACS

The work to be presented has been completed under a contract with CNES (1996-1998). The software used by CNES for analyzing the data produced by the survey satellite SPOT makes a heavy use of the Gauss-

Newton algorithm in the nonlinear least squares minimization module. A good understanding of Gauss-Newton convergence is therefore important.

The presentation will start from a state of the art survey on Gauss-Newton as of 1996, and will outline 2 major advances in the understanding of the convergence of Gauss-Newton that happened during the contract:

1. a geometric interpretation of a new sufficient condition for convergence when the control parameter is 1D. In addition, it is shown why and when, if the sufficient condition is not satisfied, bounded chaotic iterations are to be expected,
2. a new sufficient condition when the control parameter is a vector in $\mathbb{R}^n$, n arbitrary, for $m > n$ nonlinear functions. Known sufficient conditions in the literature turn out to be particular cases. Moreover, the sufficient condition is related to the condition number which measures the sensitivity of an extremal solution with respect to perturbations in the observed data.

Numerical analysis of elliptic/hyperbolic systems arising in superconductivity

C. M. Elliott

University of Sussex

We consider an elliptic equation nonlinearly coupled with either a first order conservation law or an equation of Hamilton-Jacobi type. Numerical discretisations are devised and analysed with respect to convergence and long time behaviour. The systems arise as vortex density models for Type II superconductors. Computational simulations are presented and discussed.

Complementarity Problems and Equilibrium Programming

Michael C. Ferris

University of Wisconsin

Complementarity problems arise in many practical models from engineering, economics and finance. Examples include computable general equilibria, traffic network design, option pricing and structure failure.

We will describe the mixed complementarity problem and give simple examples of how the above applications fit into this format. A description of various state of the art solvers for complementarity problems, including the PATH solver, will be given. Numerical issues relating to robustness and large scale implementation and extensions of the work to Mathematical Programs with Equilibrium Constraints will be mentioned.

Cartesian grid methods for advection-diffusion and streamfunction-vorticity equations in complex geometries

Randall J. LeVeque¹ & Donna Calhoun

¹University of Washington

We have developed a method which makes use of both finite volume and finite difference approaches on Cartesian grids to solve two-dimensional advection-diffusion equations in complex geometries. In this approach grid cells are cut by the boundary, rather than using a grid that conforms to the boundary. High-resolution methods from CLAWPACK are used for the advection part to keep steep gradients sharp. These are applied in an explicit manner that remains stable with reasonable time steps regardless of the size of small cut cells.

This approach has also been extended to solve the incompressible Navier-Stokes equations in an irregular region using a streamfunction-vorticity approach. Vorticity is advected and diffused using the advection-diffusion algorithm. No-slip boundary conditions are implemented by determining the correct flux of vorticity at the boundary in each time step using an immersed interface method.

Energy conservation by Störmer-type numerical integrators

Christian Lubich

Universität Tübingen

The Störmer/Verlet method is the most widely used numerical integrator in molecular dynamics, for a good part because of its long-time conservation of the total energy and also of adiabatic invariants such as the oscillatory energy. The long-time behaviour has previously been explained by a backward analysis which interprets the numerical solution as the "almost" exact solution of a perturbed Hamiltonian system. This explanation is only valid when the product $h\omega$ of the time step h with the highest frequency ω is very small, a situation that is often not met in practical computations.

Here we consider the energy behaviour for fixed positive $h\omega$ in the range of linear stability, for a class of nonlinear model problems with a single high frequency ω . This class includes the Fermi-Pasta-Ulam model of alternating soft nonlinear and stiff linear springs, for which we present numerical experiments. Although energy errors are $O(h^2\omega^2)$, the averages of the energy over finite time windows are preserved over very long time intervals. This is explained, and the deviation of the finite-time averages from the initial energy is explicitly quantified in terms of certain modified total and oscillatory energies which are conserved up to $O(h^2)$ for very long times. The analysis uses only the symmetry of the method, not its symplecticity.

Related results about the long-time conservation of energy hold for wider classes of symmetric numerical integrators including the trapezoidal rule, the fourth-order Numerov method, and also for dispersion-free methods such as Gautschi-type methods and the mollified impulse method which integrate the linear part of oscillatory differential equations exactly.

The talk is based on joint work with Ernst Hairer.

Krylov subspace methods for radial basis function interpolation

M. J. D. Powell¹ & A. C. Faul

¹University of Cambridge

Radial basis function methods for interpolation to values of a function of several variables are highly useful, because the matrix of the linear system of equations is nonsingular under mild conditions on the positions of the interpolation points, which is due to a closely related variational calculation. Let s^* be the required interpolant. The variational problem provides a semi-norm with the property that, given any two estimates of s^* , one can identify which estimate is better, where goodness is measured by the semi-norm distance to s^* . Further, s^* need not be available, because the answer to the question depends only on the coefficients of the two estimates and on the right hand sides of the interpolation equations. Therefore, if a line search method replaces an estimate s by $s + \alpha t$, where α is the step-length of the line search, then the optimal value of α can be calculated. Some iterative algorithms of this kind will be considered. The functions $s \equiv 0$ and $t = As^*$ occur on the first iteration, A being a linear operator such that As^* can be generated from the known values of s^* at the interpolation points. Then, after k iterations, the current s minimizes the semi-norm distance to s^* within the linear subspace that is spanned by $A^j s^*$, $j = 1, 2, \dots, k$. Some choices of A that depend on approximations

to Lagrange functions will be recommended. Usually they provide excellent accuracy in fewer than 10 iterations, even when there are huge numbers of interpolation points in general positions.

Adaptive Finite Element Discretization of Optimization Problems

R. Rannacher

Universität Heidelberg

We discuss a new approach towards error control and adaptivity for finite element discretizations in optimization problems governed by partial differential equations. By the Lagrangian formalism one obtains the first-order necessary optimality condition in form of an indefinite boundary value problem. Its stationary points are to be computed by a finite element method. The mesh adaptation is driven by residual-based a posteriori error estimates obtained by duality arguments. This approach facilitates control of the error with respect to any given quantity of physical interest. The specific feature introduced by the optimization problem is the natural choice of the error-control functional to coincide with the cost-functional of the optimization problem. In this case, the Lagrangian multiplier can directly be used in weighting the cell-residuals in the error estimator. This leads to a particularly simple and cost-efficient algorithm for adapting the mesh according to the particular needs of the optimization problem.

From good approximations on the sphere to the scattering of sound

I. H. Sloan

University of New South Wales

The focus of this talk is on how to construct good polynomial approximations (more precisely, spherical polynomial approximations) on the sphere. We might ask: can we achieve (as in the case of a circle or interval) a good polynomial approximation of a well behaved continuous function by classical interpolation at well chosen points? The known theoretical results, which are few, fail to answer the question satisfactorily, but numerical experiments suggest that the answer is: possibly, but only if the interpolation points are chosen very, very carefully; and even then the best current results (obtained recently by R Womersley) suggest that the uniform norm of the interpolation operator (i.e. the Lebesgue constant) grows roughly linearly in n , where n is the maximum degree of the spherical polynomial space.

The talk also introduces hyperinterpolation. Although requiring more information than interpolation, it is shown to be easier to implement, and to have very good, indeed in a certain precise sense optimal, properties in both theory and practice. In particular, it leads to a Lebesgue constant that grows only as $n^{1/2}$ (a result from recent joint work with R Womersley).

The talk will also consider briefly a seemingly unrelated problem, of the scattering of sound waves from a smooth 3-dimensional scatterer. It turns out that the properties of hyperinterpolation play a key role in a current analysis (in joint work with I Graham) of a fast spectral method due to L Wienert. In particular, it is crucial in this analysis that the Lebesgue constant grows more slowly than n .

Model reduction of large-scale dynamical systems

Paul Van Dooren

Catholic University of Louvain

In this talk we survey recently developed model reduction techniques for large scale dynamical systems, modelled via systems of equations of the type

$$\begin{cases} \dot{x}(t) = F(x(t), u(t)), \\ y(t) = G(x(t), u(t)). \end{cases}$$

These models are encountered in the study of control systems where $u(t) \in (\mathbb{R}^m)$

$\mathbb{R}^m$ is the input, $x(t) \in (\mathbb{R}^N)$

$\mathbb{R}^N$ is the state and $y(t) \in (\mathbb{R}^p)$

$\mathbb{R}^p$ is the output, respectively, of the system. Typically m and p are small but N can be very large. We assume that this model arises from the discretization of a continuum problem (such as finite-element models of chemical processes or mechanical systems) and hence correspond to sparse systems of equations $F(\cdot, \cdot)$ and $G(\cdot, \cdot)$.

Although the numerical simulation of such systems may still be viable for large state dimensions N , most control problems of such systems require the construction of a feedback $u(t) = K(x(t))$ which is typically of much higher complexity. In order to cope with this one uses nowadays model reduction techniques, which consist in constructing a lower order model with a much smaller state $\hat{x}(t) \in (\mathbb{R}^n)$

$\mathbb{R}^n$ which "mimics" the input/output behaviour of the original system.

We survey such techniques and put emphasis on the case where $F(\cdot, \cdot)$ and $G(\cdot, \cdot)$ are linear time-invariant, but also briefly mention recent results for the linear time-varying case as well as the nonlinear case.

Solving data fitting problems with bounded uncertainties in the data

G. A. Watson

University of Dundee

Of interest here is the fitting of a linear model to discrete data where all the data are subject to errors, and there are known bounds on these errors. It is then important that the effect of the uncertainties in the data is not unnecessarily overestimated in the fitting process. The formulation and analysis of such problems has attracted attention in the special case when the underlying criterion is the least squares norm, and here such problems are treated in a more general l_p setting. Numerical methods are considered for obtaining solutions.

Domain Decomposition Algorithms using Lagrange Multipliers

Olof Widlund¹ & Axel Klawonn

¹Courant Institute of Mathematical Sciences

Domain decomposition methods have been developed quite systematically and successfully, in particular, for conforming finite element approximations of elliptic problems. These algorithms are preconditioned conjugate gradient-type methods based on solvers for subregions and certain low-dimensional global models. In many methods the preconditioners are simply built from a large number of much smaller instances of the original finite element problem. The best results show that the number of iterations required to decrease the residual norm by a fixed factor is independent of the number of local subproblems, which form an important part of the preconditioner, and is also independent or only grows very slowly with the dimension of the local problems. These algorithms are designed with parallel and distributed computing in mind and there is now a considerable and positive experience with hard problems. Large software systems have been built based on these ideas.

In this talk, a description will first be given of two successful domain decomposition methods of Schur complement type, namely the balancing and the FETI methods. The FETI algorithm, invented and much

developed by Farhat and Roux, has the interesting feature that the continuous finite element solution is approached through a sequence of discontinuous iterates. The jumps across the interface, defined by the boundaries of the subregions are controlled by Lagrange multipliers and when accurate enough values of these dual variables have been found, then the solution on individual subregions can be computed locally. The convergence of the iteration can be monitored by observing the jumps across the interface and when they have decreased sufficiently we are close to convergence.

We have made two contributions to the further understanding of these methods. We have first shown how the FETI method can be redesigned so inexact solvers can be used for the subregions. In such an algorithm both the solution and the Lagrange multipliers are updated in each iteration step after that the problem has been recast as a saddle point problem. This work is based on earlier work by Klawonn and others on preconditioners for saddle point problems. It is interesting to note that the leading principal block of the saddle point matrix is only positive semidefinite. We have also developed new versions of the FETI algorithm for which the convergence is faster and for which existing theory, primarily due to Mandel and Tezaur, also can be improved. We have found a surprisingly simple connection between this theory and that of the balancing method. This has allowed us to simplify and unify the theory and to develop valuable tools that can assist us directly in the design of appropriate variants of the FETI method.

Abstracts of Contributed Talks

Accelerating the Limited Memory BFGS Method with Inexact Line Searches

M. Al-Baali

Sultan Qaboos University

Although the limited memory (L-) BFGS method is attractive for solving large scale optimization problems, it has a few drawbacks when applied to certain (simple and difficult) type of problems. These drawbacks are related to a given fixed number (say, m) of the stored difference vector pairs, since the L-BFGS algorithm employs exactly m BFGS updates per iteration. To avoid these disadvantages, we propose some modifications to this method so that the number of updates varies at each iteration. The modifications depend on a new criterion which measures some behaviour of the Hessian approximations. Numerical results are presented which show that the modified L-BFGS methods perform substantially better than the L-BFGS algorithm in terms of either the number of updates (which is time-consuming) or the number of function and gradient evaluations required to obtain the solutions of certain standard problems.

A spectral element approach to solve the Poisson equation

K. Amoura¹ & F Z Nouri

¹University of Annaba

We propose to solve the Poisson problem by a spectral method. A new procedure, based on the "joint method" is considered. It has been proved by Bernardi and Al that a three-dimensional problem can be reduced to a bidimensional one. However, singularity difficulties occur. To overcome these, especially in domains with corners, we use a technique based on a domain decomposition procedure. We present theoretical and related numerical results for an axisymmetric problem in fluid mechanics.

On the solution of singular perturbation problems using non-monotone methods on Shishkin meshes

Ali Ansari¹ & Alan Hegarty¹University of Limerick

Numerical methods for solving singularly perturbed problems, such as stationary convection-diffusion problems, commonly involve the use of upwind finite difference operators (i.e., one sided difference operators) together with specially adapted computational meshes such as Shishkin or Bakhvalov meshes. Upwind operators have the following advantages: they admit a maximum principle and are consequently stable; also solutions to the resulting systems of linear equations can generally be obtained by modern iterative methods within a reasonable number of iterations. On the other hand, non-monotone methods, such as central differencing or Galerkin finite element methods, while attractive because of the higher order of convergence attainable, tend to exhibit non-physical oscillations in the numerical solutions and the linear systems are known to be extremely difficult to solve. We are not concerned here with resolving the difficulties presented by the oscillations, as this has been dealt with elsewhere. Here we discuss how to make the non-monotone methods more robust by the use of preconditioners that significantly reduce the number of iterations of the linear solver.

Error estimates for finite element methods with anisotropic meshes**Thomas Apel**

TU Chemnitz

We consider partial differential equations whose solution has (at least locally) different behaviour in different space directions. Applications include problems with edge and interface singularities in diffusion dominated problems (Poisson type equations) or with boundary layers arising in singularly perturbed problems.

The idea is to reflect this behaviour of the solution in a finite element approximation by using *anisotropic meshes* with a small mesh size in the direction of the rapid variation of the solution and a larger mesh size in the perpendicular direction.

After an introduction into anisotropic finite elements we focus on local interpolation error estimates for conforming and non-conforming finite elements. These are applied to estimate the discretization error for model problems.

Error propagation in the numerical integration of solitary waves. The regularized long wave equation**A. Araújo¹ & A. Durán**¹University of Coimbra

We study the error propagation of time integrators of solitary wave solutions for the regularized long wave equation, $u_t + u_x + 1/2 (u^2)_x - u_{xxx} = 0$, by using a geometric interpretation of these waves as relative equilibria. We show that the error growth is linear for schemes that preserve invariant quantities of the problem and quadratic for "nonconservative" methods. Numerical experiments are presented.

A Nyström Method for Integral Equations on the Real Line and an Application to Scattering by Diffraction Gratings**T Arens¹, A. Meier, S.N. Chandler-Wilde & A. Kirsch**

¹Brunel University

We propose and analyse a theoretical Nyström method for a class of second kind integral equations on the real line. Convergence and stability results are presented that are uniform with respect to all kernel functions satisfying certain smoothness assumptions. The method is then applied to acoustic scattering by a diffraction grating. We prove that the method is super-algebraically convergent provided the periodic boundary is smooth enough, uniformly with respect to the period of the boundary. Numerical results illustrating this convergence rate are presented. This method will also be employed and extended to the case of a rough surface in the talk by A. Meier.

Dynamic iteration for coupled differential-algebraic systems

Martin Arnold

DLR German Aerospace Center

Multi-rate methods, multi-method approaches and dynamic iteration methods are frequently used in the time integration of coupled systems of differential equations. All these methods may get unstable if the systems are coupled by algebraic constraints. In the talk we consider the time integration of coupled differential-algebraic systems and give sufficient conditions for stability and convergence. Furthermore, preconditioning is used to fix the instability phenomenon.

Computation of a Few of The Largest Eigenvalues of Symmetric Matrices

Ran Baik¹, Karabi Datta & Yoopyo Hong

¹Honam University

In this paper we provide an iterative method to obtain a few of the largest eigenvalues and the corresponding eigenvectors of symmetric matrices. The method based on the Group Homotopy method that we have developed. The rate of convergence of this method depends on the gap of each intermediary steps where gap of a matrix is defined to be the minimum distance between distinct eigenvalues of the matrix. The Homotopy method is developed to deal with drawbacks in the existing Homotopy methods, namely, (i) the absence of any definite criterion to choose a step size that guarantees the convergence of the method and (ii) the possibility of breakdown or having a slow rate of the convergence in the presence of clustering of eigenvalues. In the course of developing the Homotopy method, we have also developed a globally convergent modified newton method that in use in each stage of the Homotopy method to guarantee the convergence of the iteration. The modified Newton method uses a stepsize control to achieve a monotone decline of the value of $\|(\alpha I - A)X\|_2$. Also, since the method preserves the special structure of matrices (for examples, Toeplitz matrices, symmetric matrices), it is suitable to obtain eigenpairs of a class of matrices which possesses some special characteristics that we might take advantage of. On the other hand, the Homotopy method maintain attractive features of the ordinary such as natural parallelism and the structure properties. Those attractive features provide another new approach to get a group of the largest eigenpairs of the matrix without calculating of other eigenvalues. On these merits, this paper is devoted to compute of the largest eigenvalues of symmetric matrices and also is analyzed with the existing methods for computing the extremal eigenvalues of the matrix.

Optimal Symmetric Cubature Formulae

Steven Bailey

University of Wales Cardiff

Just a very short and sweet introduction to the content of my PhD. Simply, what a symmetric cubature formula is and the method currently being used to optimise them.

The linear rational collocation method for PDEs

R. Baltensperger¹ & J.-P. Berrut

¹University of Fribourg

The global pseudospectral method of lines for solving hyperbolic or parabolic differential equations for a function $u(x,t)$ of the spatial variable x and the time variable t can be described as follows: One chooses interpolation points (nodes) x_i in the spatial interval, replaces u for every t by a polynomial $[u\text{tilde}]$ interpolating between the x_i 's, inserts $[u\text{tilde}]$ into the equation and collocates at the x_i 's. This leads to a system of ODEs in t that is then solved by a time marching technique. In the latter, the vectors of values of $[u\text{tilde}]$ are multiplied by differentiation matrices $\mathbf{D}$ whose entries are the derivatives of the fundamental Lagrange polynomials at the nodes.

For precise and well-conditioned interpolation, the x_i 's must be chosen in such a way that their preimages on the circle by the application $\arccos$ are almost equidistant (e.g., Chebyshev or Legendre points), which make them concentrate near the extremities of the interval. This results in ill-conditioned differentiation and highly nonnormal $\mathbf{D}$'s which for stability require smaller time steps than difference or element methods using equidistant nodes.

For the Chebyshev case, Kosloff and Tal-Ezer in 1993 suggested to shift the points toward a more regular distribution by means of a conformal map. In view of the chain rule, the corresponding change of variable results in differentiation matrices that are sums of products of the $\mathbf{D}$'s with diagonal matrices of values of derivatives of the map. These new matrices are closer to normality than the $\mathbf{D}$'s and therefore increase the timestep necessary for the stability of the time marching technique.

In our talk we will show how the same can be achieved by replacing the interpolating polynomial by some linear rational interpolant, i.e., a rational interpolant whose denominator is independent of the interpolated function.

Dynamics of the Theta Method

G. J. Barclay¹, D. F. Griffiths & D. J. Higham

¹University of Strathclyde

The Theta method is a family of ODE timestepping formulas parameterized by a value $\theta \in [0,1]$. Choosing $\theta = 0, 1/2, 1$ gives forward Euler, the trapezoidal rule, and backward Euler, respectively. Values in the range $1/2 \leq \theta \leq 1$, where the method is A-stable, are often used in practice.

In this talk we will show that the simple structure of the Theta method makes its long term dynamics amenable to detailed analysis. We will look at spurious period two solutions arising on nonlinear problems, showing that, for small timesteps, these solutions are generically unstable for $\theta < 1/2$ and stable for $\theta > 1/2$. We will then focus on particular classes of problems and make direct connections between the existence and stability of period two solutions and the dynamics of the Theta method. The results will be illustrated with numerical examples.

More Accurate Bidiagonal Reduction for Computing the SVD

Jesse L. Barlow

The Pennsylvania State University

Bidiagonal reduction is the preliminary stage for the fastest stable algorithms for computing the singular value decomposition. However, the best known error bounds on bidiagonal reduction methods on any matrix are of the form

$$A + \delta A = UBV^T,$$

$$\|\delta A\|_2 \leq \varepsilon_M f(m,n) \|A\|_2$$

where B is bidiagonal, U and V are orthogonal, ε_M is machine precision, and $f(m,n)$ is a modestly growing function of the dimensions of A .

A pre-processing technique used by Demmel and Veselić [SIAM J. Matrix Anal. Appl., 13:1204-1243, 1992] is to compute the orthogonal factorization with column pivoting to obtain

$$A = Q \begin{pmatrix} C^T \\ 0 \end{pmatrix} P^T$$

where Q is orthogonal, C is lower triangular, and P is permutation matrix. Those authors then applied the Jacobi SVD algorithm to C . Since the Jacobi SVD algorithm can be implemented to obtain an SVD triplet (U, Σ, V) such that

$$C + \Delta C = U \Sigma V^T$$

where

$$\|\Delta C e_j\|_2 \leq \varepsilon_M g(n) \|C e_j\|_2$$

and since the matrix C is well-conditioned after column scalings, the resulting procedure tended to obtain more accurate singular value and vectors of C than would be expected from algorithms that require a bidiagonal reduction.

The work described here reopens this issue by obtaining a conditional columnwise error bound on the bidiagonal reduction of C . If we have that, there is now a good menu of algorithms that obtain the singular values of a bidiagonal matrix to relative accuracy. For that reason, we propose a Givens-based bidiagonal reduction procedure is proposed for matrices of the form C that satisfies

$$C + \Delta C = U (B + \Delta B) V^T,$$

where δB is bounded *componentwise*, δC satisfies a columnwise bound that is nearly as good as that for the Jacobi algorithm, and U and V are orthogonal to nearly working precision. The only additional operations required are for an $O(n^2)$ flops pre-processing step, and those for using Givens rotations instead of Householder transformations to compute the matrix V . If fast rotations are used, the flop count of this new routine is only $O(n^2)$ flops greater than that for the Householder based algorithm of Golub and Kahan [SIAM J. Numer. Anal. Ser. B, 2: 205-224, 1965].

A Study of Moving Mesh Methods as Applied to a Thin Flame Propagating in a Detonator Delay Element

T. Basebi¹ & R.M. Thomas

¹UMIST

We study moving mesh methods as applied to a one-dimensional (time dependent) detonator delay element problem. We consider moving mesh methods based on the equidistribution principle. A number of adaptive mesh methods have been widely used recently to solve time dependent partial differential equations having

large solution gradients. Significant improvements in accuracy and efficiency are realised by adapting the nodes (mesh points) so that they are concentrated about areas of large solution variations. Each system of equations for the moving mesh methods is solved in conjunction with the detonator problem. In this paper a resulting ordinary differential equation system is solved using the double precision version of the stiff ordinary differential equation solver DASSL. We present an alternative choice of a weighted root mean square norm for DASSL (for mixed error test) in order to solve the detonator element problem. The numerical results clearly demonstrate that the moving mesh methods are capable of tracking the deflagration wave as it travels down the detonator delay element more accurately than a fixed mesh method. We also give a brief discussion explaining why some of the moving mesh methods fail to solve the detonator problem. In line with this, we give some plots to show how the smoothness in change of stepsize and the size of the stepsize ratio can affect how efficiently a moving mesh method solves the detonator problem.

The adaptive solution of singularly perturbed boundary value problems using a posteriori error estimation

G. Beckett¹ & J. A. Mackenzie

¹University of Strathclyde

In this talk, I will describe a class of procedures for generating a posteriori error estimates for elliptic PDE's via the solution of local auxiliary problems, which are commonly posed with either Dirichlet or Neumann boundary conditions. By considering a model singularly perturbed reaction-diffusion problem - often called a weak diffusion problem - a comparison will be made between these two strategies in the context of grid selection.

A matrix for determining lower complexity barycentric representations of rational interpolants

J.-P. Berrut

University of Fribourg

Let $\mathfrak{R}_{mn}$ be the set of all rational functions with numerator degree $\leq m$ and denominator degree $\leq n$. We want to find a rational function $r \in \mathfrak{R}_{mn}$, $m+n = N$, $m \geq n$, interpolating $N+1$ given function values $\{f_k\}_{k=0}^N$ in $N+1$ real and distinct interpolation points $\{x_k\}_{k=0}^N$. Starting from the fact that any such r can be written in barycentric form, we have noticed in 1997 that the vectors of *weights* $\{u_k\}_{k=0}^N$ of such representations must satisfy degree diminishing conditions in the form of homogeneous equations. Taken together, these conditions determine the kernel of a matrix made of a $m \times (N+1)$ Vandermonde for the conditions for the denominator on top of a $n \times (N+1)$ Vandermonde for the numerator. By means of triangulation of this matrix, we have given an experimentally stable, $O(m^2 + mn + n^3)$ algorithm for finding the weights (if r exists).

Besides all its advantages, the barycentric representation has the drawback that its evaluation at a point x requires about twice as many flops as the canonical representation. To improve on this, at least partially, we suggest to change the rational form in such a way that merely $M < N$ interpolation conditions are guaranteed by the barycentric formula. This way, only M weights are to be determined, and evaluation of r requires about $2M$ flops. The weights $\{u_k\}_{k=0}^M$ - if they exist - now span the kernel of a matrix made of three submatrices on top of one another, a $(M-n) \times (M+1)$ Vandermonde for the degree conditions of the denominator, a $(M-m) \times (M+1)$ Vandermonde for the numerator and a $(N-M) \times (M+1)$ Löwner (or divided difference) matrix for the interpolation conditions at the points without barycentric weight.

In our talk, we will describe an algorithm for finding lower complexity representations of r by means of this matrix and present results obtained in numerical computations.

Iterative multiscale methods for state estimation

Luise Blank¹, Thomas Binder, Wolfgang Dahmen & Wolfgang Marquardt

¹RWTH Aachen

Real-time state estimation is accomplished by the solution of an appropriately posed optimization problem on a receding horizon. Uncertainties in the model are accounted for by additive correction terms to be estimated simultaneously. The essential problem is that the available computation time is not known beforehand. Therefore, we propose a multiscale approach based on wavelets. It shall provide a coarse approximation after a very short time and upgrades the initial solution in each refinement step up to a given error improvement with proportional costs.

Discrete compactness for edge elements

Daniele Boffi

Università di Pavia and Penn State University

The edge elements are widely used for the approximation of the Maxwell's system. In the two-dimensional case the known families of edge elements are isomorphic to the well-studied Raviart-Thomas or Brezzi-Douglas-Marini elements (the so-called face elements), which have been introduced for the approximation of the space $H(\text{div})$. In the three-dimensional case edge and face elements still have some analogies but are no longer the same. We present some results concerning the approximation of the eigenvalue problem associated with the Maxwell's system. During the last two years the study of Maxwell's equations has been carried out by several authors. This led to a deeper knowledge of their properties, in particular of the regularity and singularity of the solution. The analysis of the convergence of the eigenmodes is carried out by writing the discrete eigenvalue problem in mixed form and by making use of recent results on the approximation of mixed eigenvalue problems. These are related to the construction of a so-called Fortin operator and to the study of its properties. Moreover we show that the edge elements satisfy a discrete compactness property introduced by Kikuchi. This constitutes the first general proof of convergence for the approximation of the Maxwell's eigenproblem using the edge elements.

Introduction to the Numerical Treatment of Stochastic Delay Differential Equations

Evelyn Buckwar¹ & Christopher T. H. Baker

¹University of Manchester

We are concerned here with stochastic delay differential equations (SDDEs), which generalise both deterministic delay differential equations and stochastic ordinary differential equations. This class of problems is of practical interest, e.g. in population dynamics and robotics.

Let $(\Omega, \mathcal{A}, P)$ be a complete probability space with a filtration $(\mathcal{A}_t)$ satisfying the usual conditions. Let $W(t)$ be the 1-dimensional Brownian motion given on this space. Let $0 = t_0 < T < \infty$ and consider the SDDE with one fixed lag τ :

$$\left. \begin{aligned} dX(t) &= f(t, X(t), X(t-\tau)) dt + g(t, X(t)) dW(t), & t \in [0, T] \\ X(t) &= \Psi(t), & t \in [-\tau, 0] \end{aligned} \right\} \quad (\text{the equation})$$

where $\Psi(t)$ is an $\mathcal{A}_{t_0}$ -measurable $C([- \tau, 0], \mathbb{R})$ valued random variable such that $E \|\Psi\|^2 < \infty$. The SDDE () is interpreted in the Itô sense. If g does not depend on X the equation has *additive noise*, otherwise it has *multiplicative noise*. A unique strong solution to Equation () exists, if f and g satisfy Lipschitz conditions and a linear growth bounds.

We address the principal issues involved in progressing to the numerical treatment of Equation (). We will discuss some methods for approximating strong solutions of the SDDE and we will present numerical results.

Modified Newton's Method: Convergence Issues and Properties

M. Isabel R. F. Caiado¹, M. Teresa Monteiro & Edite M. G. P. Fernandes

¹Universidade do Minho

The best known classical method to solve nonlinear unconstrained minimization problems is Newton's method. The main goal of this work is to propose a modification to Newton's method to overcome the singularity of the coefficient matrix and the non-descentness of the Newton direction. The basic idea is to combine steepest descent and Newton directions. We establish conditions for a local q -quadratic convergence rate as well as for a global convergence. As far as properties are concerned, conditions for positive definiteness of the coefficient matrix are established. It is also proved that the modified search direction is gradient-related and satisfies a fraction of the optimal decrease. Finally we prove that the new direction is bounded away from orthogonality to the negative gradient.

Numerical solution of 2-phase Stefan problems

Jim Caldwell

City University of Hong Kong

Melting and solidification problems arise in numerous important areas of science, engineering and industry. The classical phase-change problem is that of melting and solidification via the conduction of heat, which is referred to as the Stefan problem in the literature. For such problems the boundary of the domain is not known in advance and so the solution involves solving the heat conduction or diffusion equation in an unknown region which has also to be determined. A wide range of techniques have been developed to solve the Stefan problem and a good account of analytical solutions is given by Hill [1]. However, numerical techniques are more commonly used and a useful account of these is given by Crank [2]. One approach to the solution of Stefan problems is the so-called front-tracking method and in this approach the phase boundary is continuously tracked. The example which is used in this work is the heat balance integral method (HBIM) which explicitly tracks the motion of isotherms (the phase change being one of them). One can also employ finite-difference schemes and let the grids deform as the phase boundary moves. These techniques provide a method of tracking the phase front explicitly. In past work (see Caldwell and Chiu [3,4]) the simple front-tracking method, namely the HBIM, has been used to solve one-phase solidification problems. In this work the method is extended to two-phase Stefan problems which arise when sub-cooling effects are taken into account. As a result numerical results are presented for the two-phase spherical and cylindrical problems for a range of parameters and the effect of the variation of these parameters on the solidification process is studied.

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Avoiding the order reduction of Runge-Kutta methods when integrating boundary value problems for autonomous linear partial differential equations with nonhomogeneous terms**M. P. Calvo¹ & C. Palencia**¹Universidad de Valladolid

A commonly used approach when solving evolutionary problems in partial differential equations is the method of lines. First, the partial differential equation is discretized in space and then, the resulting system of ordinary differential equations is time integrated. It is well known that when the resulting ODE system is integrated with a Runge-Kutta method, the order reduction phenomenon occurs. In this talk we present a technique which avoids the order reduction when a Runge-Kutta method is used for the time integration of the semidiscrete equations associated to boundary value problems for autonomous linear partial differential equations with nonhomogeneous terms. Numerical results are presented to illustrate that the expected orders are obtained.

Approximating the Logarithm of a Matrix with Variable Accuracy**Sheung Hun Cheng¹, Nicholas J. Higham, Charles S. Kenney & Alan J. Laub**¹Centre for Novel Computing, University of Manchester

A standard way to compute the logarithm of a matrix is the inverse scaling and squaring method, which repeatedly takes square roots to bring the matrix close to the identity, then applies a direct approximation such as a Padé approximation, and finally rescales. We develop an extension of the method with two key properties. First, it aims for a user-specified accuracy in the computed logarithm, requiring less work when more modest accuracy is requested. When full accuracy is required, our method becomes a new implementation of the original inverse scaling and squaring method. Second, our method can be implemented using only the basic building blocks of matrix multiplication, LU factorization and matrix inversion. The method is therefore attractive for high-performance computation.

Towards highly accurate numerical approximation through defect correction and domain decomposition**A.S. Chibi**

University of Annaba

Our aim in this article is to combine the techniques of defect correction and domain decomposition to obtain highly accurate numerical approximation for second order elliptic boundary value problems on a disc. The basic solution is computed using the Schwarz domain decomposition procedure and bilinear Galerkin finite element approximation on each subdomain to get a second order accurate basic solution in higher order discrete Sobolev norms. The defects are then computed using high order interpolation polynomials (Lagrange polynomials or splines) to get as many $O(h^2)$ corrections as possible.

On the accuracy of difference schemes on nonuniform grids**Raimondas Ciegis**

Vilnius Gediminas Technical University

The boundary value problem for the second order difference equation

$$u_{xx} + q(x)u = f(x)$$

is solved numerically on the nonuniform grid. Three difference schemes are constructed. It is proved that solutions of these schemes have the second order of accuracy in the uniform norm. The results of numerical experiments are used to compare the efficiency of the schemes.

Factorized Quasi-Newton structured techniques for nonlinear least squares problems

M. Fernanda P. Costa¹ & Edite M.G.P. Fernandes

¹Universidade do Minho

In this talk we consider Quasi-Newton structured methods for finding a local solution to nonlinear least squares problems. These techniques take into account the special structure of the problem using Quasi-Newton updates to approximate only the second part of the Hessian. In order to maintain positive definiteness of the coefficient matrix, guaranteeing a descent search direction for the objective function, a factorized correction matrix is added to the first part of the Hessian which depends on the Jacobian.

To deduce the updating formula for the factorized matrix we use the least change secant update technique, minimizing the change in the solution to the model under the Frobenius norm, subject to satisfying a specific secant condition. Five different least change formulations are considered. A sizing strategy is also included to take the updating matrix to converge to zero in zero residual problems.

Numerical results are included for a variety of well known problems and compared with Gauss-Newton and other Quasi-Newton structured techniques.

Up-wind based schemes in the simulation of free surface flows

J. A. Cuminato¹, A. Castelo Filho, V. G. Ferreira & M. F. Tome

¹University of Sao Paulo

The convective terms in the Navier-Stokes equations are primarily responsible for many of the complex flow phenomena. They are also the major cause of numerical difficulties, and several techniques for treating these terms have been proposed over the last years. In particular, the finite difference approximation to the derivatives deserves special attention if one seeks to obtain accurate and stable schemes for realistic problems. The usual central difference scheme may lead to unphysical oscillatory behaviour in regions of the flow where convection dominates diffusion while the first order upwind ensures stability but introduces false diffusion. The QUICK scheme combines the accuracy of quadratic interpolation with stability to obtain diffusion free and high order numerical schemes. Recently Zhu introduced a new scheme for treating convection dominated flows called HPLA. This scheme has the property of combining the high order accuracy of the QUICK with an anti-diffusive term correcting the upwind scheme. In this work we present test results for the above four numerical schemes for the simulation of free surface flows using the SMAC technique in the GENSMAC method.

Error Reduction in Matrix Vector Multiplication Method

Mohammad Taghi Darvishi

Razi University

To reduce the roundoff error in computing derivatives using Chebyshev collocation methods (CCM) a new preconditioning method is investigated. Also for accuracy enhancement of differentiation a domain decomposition approach is used. Error analysis shows that for this domain decomposition method error reduces proportional to the length of subintervals. Numerical results show that using domain decomposition and preconditioning simultaneously, gives super accurate approximate values for first derivative of the function and good approximate values for moderately high derivatives. Finally an alternative domain decomposition method and preconditioning schemes are investigated for computing high order derivatives. Error analysis shows that using the proposed domain decomposition method, as the number of subdomains increase, numerical solution closes to the exact solution. Other aspects of the domain decomposition method like CPU time, memory allocation and smallness of entries of differentiation matrix are also studied.

Generating Test Matrices for the One- and Two-Sided Jacobi Methods

Philip I. Davies¹ & N. J. Higham

¹Manchester University

For a symmetric positive definite matrix the relative error in the eigenvalues computed by the two-sided Jacobi method is bounded in terms of the condition number of the matrix scaled to have unit diagonal. Similarly, for a general matrix the relative error in the singular values computed by the one-sided Jacobi method is bounded in terms of the condition number of the matrix scaled to have rows or columns of unit-2 norm. We show how to generate random matrices having these scalings and given eigenvalues and singular values, respectively. For the two-sided Jacobi method we apply an algorithm of Bendel and Mickey for generating random correlation matrices, with an improved formula for the rotations. We show how to modify the algorithm to generate matrices for the one-sided Jacobi method. Using these test matrices we show empirically that the forward error bounds for the one- and two-sided Jacobi methods are sharp.

Frequency domain electromagnetic scattering from a thin wire

P J Davies¹, D B Duncan & S A Funken

¹University of Strathclyde

The computation of the current induced on a straight thin wire antenna by an incident time-harmonic electromagnetic field is a problem with a long history. Under suitable assumptions the current $u(z)$ flowing axially along a wire of unit length and radius a can be shown to satisfy the integro-differential equation (IDE)

$$-(d^2/dz^2 + \omega^2) \int_0^1 K(z-z') u(z') dz' = f(z),$$

where f is proportional to the axial component of the incident electric field, ω is the incident field frequency, and the kernel K depends on the particular approximation used.

Typically the "reduced kernel" form of the problem is used for numerical computations - however this kernel is nonsingular and the resulting IDE is ill-posed. Hence the numerical solution is meaningless unless the smallest space grid size used in its discretisation is large compared to the radius of the wire.

In contrast, it is known that the IDE with the more complicated "exact kernel"

$$K(r) = \int_0^\pi \frac{d\theta}{\exp(-i\omega \sqrt{r^2 + 4a^2 \sin^2 \theta})} d\theta.$$

$$4\pi^2 \sqrt{r^2 + 4a^2 \sin^2 \theta}$$

is well posed in the sense that the solution u depends continuously on the data f . We investigate solutions of this form of the IDE, looking at various Galerkin and collocation schemes (on uniform and adaptive meshes). Evaluating the exact kernel function can be a major problem in its own right, and so carrying out the matrix assembly can take a lot of CPU time.

On a multistep method approximating a linear sectorial evolution equation

Nicoletta Del Buono¹ & A. T. Hill

¹Università di Bari

Many problems encountered in applications, e.g. the linear and nonlinear heat equation, nuclear reaction dynamics, the Navier-Stokes equation or other convection-diffusion equations can be modelled in the abstract form $u_t + Au = f(t, u)$, $t \geq 0$, where A is a sectorial operator on a Banach space X and it generates the analytic semigroup e^{-At} . In a dynamical context, it is useful to consider the approximation of the system by a numerical semigroup and for a q -step multistep method this semigroup is defined on X^q . In this preliminary work we restrict our attention to the simpler linear sectorial equation $u_t + Au = 0$, $t > 0$ and to the approximation of e^{-At} by the numerical semigroup generated by a multistep method. Improving previous work by Hill and Süli, under certain assumption, we derive our optimal order error estimate for our approximation to e^{-At} .

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Least squares data smoothing by non-negative divided differences

I. C. Demetriou

University of Athens

A univariate function that has a non-negative m -th derivative is measured on a finite mesh of n abscissae. If unsmooth changes are observed in the m -th order divided differences of the measurements, they are usually attributed to errors due to the measuring process. We consider the calculation that makes the least squares change to the data subject to non-negative divided differences of order m , where m is a prescribed positive integer. This is a structured quadratic programming problem that can be solved by the following special method that is faster than general procedures. First calculate an initial approximation that comes close to the optimum in $O(m \cdot 2n)$ computer operations. Then, use this approximation as the starting point of a quadratic programming algorithm that completes the calculation of the optimum in the dual space. The quadratic programming algorithm avoids small step lengths along the dual search direction and automatically adjusts the tolerance that defines β_{small} . Also, it utilizes QR factorization and updating procedures efficiently and

avoids fill-in by applying suitable Givens rotations to compact storage arrays. A computer program has been written and numerical results illustrate the method and indicate the efficiency of this approach.

An efficient spectral method for nonlinear wave equations

Tobin A. Driscoll¹ & Bengt Fornberg

¹University of Colorado, Boulder

Spectral methods for nonlinear wave equations such as KdV and NLS deliver high accuracy in space. To exploit this situation efficiently, one must use a high-order time discretization while avoiding the usual severe stability restrictions. We investigate a "partially implicit" approach based on combined Adams-Bashforth and Adams-Moulton formulas. Only the stiff (dispersive) linear term is treated implicitly, so the resulting combination is essentially explicit. By selecting different integrators within the method of lines, we get high accuracy where possible while maintaining stability where necessary. The method compares favorably to high-order alternatives and is far more efficient than the usual second-order time discretizations.

Sparse preconditioning of dense problems from electromagnetic applications

Iain Duff¹, Bruno Carpentieri & Luc Giraud

¹RAL and CERFACS

We compare different preconditioning techniques in connection with Krylov methods for the solution of large dense complex symmetric non-Hermitian systems arising in computational electromagnetics. Both implicit and explicit preconditioners are considered, and we emphasize sparse approximate inverse methods. We examine issues such as the determination of the sparsity structure for the preconditioner and also the approximation of the operator which we wish to precondition. We explore some interesting issues which do not occur if the operator was sparse and show that the relative performance of the preconditioners is different from what would be expected in that case. We illustrate our results by runs on test problems from electromagnetics.

Approximating a convolution model of phase separation

D. B. Duncan¹, M. Grinfeld & I. Stoleriu

¹Heriot-Watt University

We examine issues involved in developing numerical approximations of the integro-differential equation (IDE)

$$u_t = \sigma \int_{\Omega} J(x-y) (u(y,t) - u(x,t)) dy + f(u)$$

where $\Omega \subseteq \mathbb{R}$, $\sigma > 0$, $f(u)$ is bistable (for example $f(u) = u - u^3$), $J \geq 0$, $J \in L^1$ and $J(-x) = J(x)$. This IDE has been proposed as a model of phase separation, and is a non-local analogue of the usual Allen-Cahn reaction-diffusion equation

$$u_t = \sigma \Delta u + f(u)$$

where the Laplacian differential operator is replaced by a convolution integral operator. Although the convolution operator acts to smooth the solution (to reduce spatial nonuniformity), the IDE can have discontinuous transient and steady state solutions, giving rise to some interesting numerical problems.

GMRES Convergence Bounds, Estimates, and Restarts

Mark Embree

Oxford University Computing Laboratory

What matrix properties govern convergence of the GMRES algorithm for solving non-symmetric linear systems of equations? Three popular bounds are based on the eigenvalues (with eigenvector information), the field of values, and the ε -pseudospectra of the coefficient matrix. To understand the relative merits of these bounds, we present six examples illustrating their success and failure, and demonstrate that eigenvalue and field of values bounds can be improved to cope with low dimensional non-normality.

The analytic relationship between the pseudospectra, eigenvalues and eigenvectors, and the field of values suggests that applying the pseudospectral bound to the ε -pseudospectrum for several values of ε can describe multiple phases of GMRES convergence. Unfortunately, this bound's utility is hampered by the expense of computing pseudospectra for large, sparse matrices. We show that convergence estimates are obtained by computing this bound using the pseudospectra of the upper Hessenberg matrix generated during the GMRES iteration.

Roots of the GMRES residual polynomial can be identified with particular pseudospectral sets; this connection informs analysis of restarted GMRES. We argue that for significantly non-normal matrices, GMRES(k) may outperform GMRES(l) when $k < l$. This phenomenon is illustrated with several computational examples.

Multiple shooting for index-one differential-algebraic problems using a dichotomically stable integrator

Roland England¹, René Lamour & Jesús López Estrada

¹The Open University

It has previously been established that dichotomic stability is important when solving stiff boundary-value problems in ordinary differential equations, when sharp boundary layers may occur at each end of the interval. A variable step-size, dichotomically stable, integrator for ODEs has been implemented using the 3-stage, fourth-order, Lobatto IIIA formulae. By elimination of the value at the intermediate stage, these may be written as a single formula:

$$\mathbf{X}_{i+1} - \mathbf{X}_i - h \left[\frac{1}{16} \mathbf{X}_{i+1}' + \frac{1}{23} \mathbf{F} \left\{ \frac{1}{12} (\mathbf{X}_{i+1} + \mathbf{X}_i) - \frac{1}{18} h(\mathbf{X}_{i+1}' - \mathbf{X}_i') \right\} + \frac{1}{16} \mathbf{X}_i' \right] = 0,$$

where the system of ODEs is written as $\mathbf{x}' = \mathbf{F}(\mathbf{x}) \in \mathbb{R}^n$. An explicit, 4-step, third-order, extrapolation formula is used, both as a predictor, and to provide a local error indicator. This has the correct asymptotic behaviour, both for small and for large step sizes.

For differential-algebraic equations of the form $\mathbf{F}(\mathbf{x}', \mathbf{x}, t) = 0 \in \mathbb{R}^n$, it is not possible to eliminate the value at the intermediate stage. The Lobatto IIIA formulae must be solved for the derivatives at the off-step point and at the end of the step, for each integration step. The Newton iteration matrix is then non-singular for an index-one system. Predictors are also needed for the derivatives, and at the off-step points. The Lobatto IIIA formulae have the advantage, over a Gaussian method, that the order is the same for both differential and algebraic variables, which may be treated identically.

The ODE integrator (SYMIRK) has been adapted in this way, for the solution of index-one differential-algebraic systems. The resulting integrator (SYMDAE) has been inserted into the multiple-shooting code (MSHDAE) developed by R. Lamour for differential-algebraic boundary-value problems. Tests on a few stiff

boundary-value problems have shown that, at least in some cases where the standard BDF integrator in MSHDAE fails to integrate across the interval of interest, the dichotomically stable integrator SYMDAE encounters no difficulty. What is more, the modified version of MSHDAE produces an accurate solution in such cases, and within limits imposed by computer word length, the efficiency of the solution process improves with increasing stiffness.

Feasible weight functions for Generalised quadrature methods

Gwynne A. Evans

De Montfort University

Recent methods for the numerical evaluation of integrals of the form

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

where ω is large, and g is an oscillatory kernel typified by $\sin$, $\cos$ or J_n , have been the subject of considerable recent research. The regular problem with $q(x) = x$ and $g = \sin$ or $g = \cos$ has been well solved with high order stable methods being available. A powerful method is to use Lagrange's identity

$$uLw - wMu = Z'(u, w)$$

as a basis for generating a quadrature rule for a given weight function $w(x)$, where $w(x)$ satisfies $Lw = 0$.

Not all such weight functions yield stable formula, and a theorem is proved to establish conditions for a formula to be valid to machine accuracy. Discontinuities in f or its derivatives also affect the method and are considered. These theorems are demonstrated in practice, and the conditions are shown to hold for all the irregular oscillatory quadrature rules so far investigated.

Reliable and Accurate Software for Evaluating the Complex Arctangent Function

Thomas F. Fairgrieve¹, T. E. Hull & Ping Tak Peter Tang

¹Ryerson Polytechnic University

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. Unfortunately, this is not true for the case of complex-valued elementary functions. It is not difficult to find faults in the software currently distributed by some computer manufacturers and numerical library producers.

In this talk, I will discuss the complex arctangent function and will reveal previously unguarded pitfalls. The strategies that we have used to circumvent them will be explained and a new algorithm will be presented.

Optimizing Distillation Columns

Roger Fletcher

University of Dundee

A new way of modelling a distillation column is presented which considerably reduces the number of variables and equations. The problem of finding good initial approximations is also considered. A new concept of a "homogeneous column" is described, and it is shown how solutions of such a column are more readily obtained, and enable good initial approximations to be obtained to the true column.

Numerical experiments are described. It is shown that the AMPL modelling language has proved very effective for this purpose, not least because it automatically provides first and second derivatives of all nonlinear functions that are involved.

Analysis of Fractional Differential Equations

Neville J Ford¹ & Kai Diethelm

¹Chester College

We discuss existence, uniqueness and structural stability of solutions of nonlinear differential equations of fractional order. The differential operators are taken in the Riemann-Liouville sense and the initial conditions are specified according to Caputo's suggestion, thus allowing for interpretation in a physically meaningful way. We investigate in particular the dependence of the solution on the order of the differential equation and on the initial condition and we relate our results to the selection of appropriate numerical schemes for the solution of fractional differential equations.

Staggered time integrators for wave equations

Bengt Fornberg¹, Michelle Ghrist & Tobin Driscoll

¹University of Colorado

We consider variations of the Adams-Bashforth, backwards differentiation, and Runge-Kutta families of time integrators to solve systems of linear wave equations on uniform, time-staggered grids. These methods are found to have smaller local truncation errors and to allow larger stable time steps than traditional nonstaggered versions of equivalent orders.

A scalable algorithm for heat integrated process synthesis

E. S. Fraga¹ & K. I. M. McKinnon

¹University College London

Automated optimal chemical plant design, or process synthesis, is difficult due to the size and complexity of the underlying optimization problem. A process design consists of a sequence of processing units together with the operating conditions and the interconnections between the units. When heat integration, for energy efficiency, is included, the complexity of the problem increases significantly. For early design, this imposes severe restrictions on the use of automated tools. This paper describes an extension to the Jacaranda process synthesis package. By careful use of discrete distributable quantities, a polynomial time optimization algorithm for heat integrated process synthesis has been developed. Together with improved visualization techniques, the resulting implementation is robust and can generate energy efficient processes easily and efficiently.

Linearly implicit Runge-Kutta methods for advection-reaction-diffusion equations

Javier de Frutos¹, M.P. Calvo & J. Novo

¹Universidad de Valladolid

We construct two variable-step linearly implicit Runge-Kutta methods of orders 3 and 4 for the numerical integration of the semidiscrete equations arising after the spatial discretization of advection-reaction-

diffusion equations. We study the stability properties of these methods giving the appropriate extension of the concept of L-stability. Numerical results are reported when the methods presented are combined with spectral discretizations. Our experiments show that the methods, being easily implementable, can be competitive with standard stiffly accurate time integrators.

Numerical Simulation of Reaction Diffusion Systems

M. Ganesh¹, M. A. J. Chaplain & I. G. Graham

¹University of New South Wales

This work proposes and implements a spectral method of lines approach to the numerical simulation of pattern formation in reaction diffusion systems on spherical surfaces, for example those arising in tumour invasion models. The main interest is to study the *diffusion driven instability* and in particular to identify spatial patterns which evolve in practice from unstable homogeneous steady states.

Our numerical method consists of a method of lines approach with the spatial dependence modelled using surface spherical harmonics. The resulting system of ordinary differential equations are solved by a stiff solver. The exponential convergence of spherical harmonic approximation allows us to deal with relatively small systems of ordinary differential equations (typically of order 100 in size) and simulations take a few seconds on an up-to-date computing platform. A key point in the implementation is the fast implementation of the reaction-kinetics using fast Fourier transforms.

Stability and Stabilization of some Mixed Finite Element Methods

Izaskun Garrido¹ & D F Griffiths

¹University of Dundee

Babuska and Narasimhan(CMAME, 140:183-199,1997) introduced two mixed finite element approximations of a model system of first order ODEs in order to provide a simple introduction to the consequences of LBB instability. We pursue these examples further and a) illustrate more precisely how the convergence rate depends on the smoothness of the data in both stable and unstable cases and b) introduce and report on stabilizations of the unstable method.

Numerical simulation of mixing in weakly nonhomogeneous viscous fluids

Dimitri V. Georgievskii

The Moscow State University

Stability of weakly nonhomogeneous viscous and viscoplastic flows with respect to low disturbances is investigated. To analyse decay and growth of initial disturbances, the numerical sufficient estimates based on variational inequalities in various functional spaces are obtained. Quite arbitrary incompressible nonsteady flow of homogeneous viscous fluid in 3D domain is chosen as non-disturbed deformation process. Energetical analysis of perturbations evolutions in the system may be one of steps in research of mixing process both in Newtonian and non-Newtonian media.

Splitting Methods for Mixed Hyperbolic-Parabolic Systems

A. Gerisch¹ & R. Weiner

¹Martin-Luther Universität Halle-Wittenberg

We study the numerical solution of a system of PDEs arising in the modelling of tumour induced angiogenesis and of other processes driven by chemotaxis. We employ the method of lines approach and our main goals are to obtain an efficient, stable and robust algorithm for the simulation of the system which preserves the non-negativity of the solution of the PDE in the numerical solution. The latter is not guaranteed for standard numerical methods. The method of lines leads us to a two step procedure to ensure non-negativity. We approximate the spatial derivatives in the PDE system (finite differences with flux limiter) such that an ODE system is obtained with a non-negative solution in the first step. In the second step, we solve this large and stiff system by an appropriate splitting scheme using explicit and linearly implicit methods in a suitable combination in order to ensure non-negativity and efficient computation of the solution. Numerical results are presented.

On the numerical solution of Volterra integral equations of the second kind by a spline based method

Laura Gori¹ & Elisabetta Santi

¹University of Rome "La Sapienza"

In this communication we shall present a method for the numerical solution of a Volterra integral equation of the second kind, with weakly singular convolution kernel $K(x-s)$:

$$y(x) = f(x) + \int_a^x K(x,s)g(x,s,y(s))ds, \quad x \in [a,X] \quad (1).$$

Exploiting some useful features of quasi-interpolatory splines, we construct a sequence $\{y_n\}$ of approximations of the solution of (1), and analyze its convergence property. Besides some theoretical results, a few numerical examples showing the efficiency of the method, will be displayed.

An iterative active-set method for large-scale non-convex quadratic programming

Nick Gould¹ & Philippe Toint (FUNDP)

¹Rutherford Appleton Laboratory

We consider an active-set method for solving large-scale quadratic programming problems for which there is no requirement that the objective function be convex. The methods are iterative at two levels, one level relating to the selection of the current active set, and the second due to the method used to solve the equality-constrained problem for this active set. A preconditioned conjugate gradient method is used for this inner iteration, with the preconditioner chosen especially to ensure feasibility of the iterates. The preconditioner is updated at the conclusion of each outer iteration to ensure that this feasibility requirement persists. The well-known equivalence between the conjugate-gradient and Lanczos methods is exploited when finding directions of negative curvature. Preliminary numerical results of an implementation of this method will be given.

Analysis of iterative, collocation and projection methods

Lechoslaw Hacia

Poznan University of Technology

Iterative methods with corrections are considered. Presented corrections can be determined as projections or interpolation polynomials. Proposed theory lead to iterative-projection and iterative-collocation methods. In particular, considered algorithms to solve different class of integral equations (Hammerstein and Volterra-Fredholm type) are applied. The convergence is proved and error estimate is established. Comparison of presented methods by numerical examples is made.

Exploiting hyper-sparsity in the revised simplex method

Julian Hall¹ & Ken McKinnon

¹University of Edinburgh

When solving large sparse linear programming (LP) problems, a typical implementation of the revised simplex method with a sparse factorisation of the basis matrix avoids the prohibitive cost of the standard simplex method or the revised simplex method with the explicit inverse of the basis matrix. In significant classes of LP problems, in particular those with a near or pure network structure, there is little or no fill-in in the factors of the basis matrix. For such very sparse problems, this paper illustrates how the computational cost of a commercial-quality implementation of the revised simplex method is dominated by operations involving zero values. Techniques by which this hyper-sparsity may be exploited are described. It is demonstrated that these techniques result in a computational performance which is vastly superior to that of at least one major commercial implementation of the revised simplex method. The extent to which the performance approaches that of a dedicated network LP solver is also examined.

Adaptive finite element solution of electrochemical problems at microelectrodes

Kathryn Harriman¹, David Gavaghan, Paul Houston & Endre Süli

¹Oxford University Computing Laboratory

Electrochemical sensors are used in a wide range of applications (from internal combustion engines to blood gas analysis) for measuring concentrations and reaction rates of chemical substances and processes. Mathematically the problem can be reduced to that of finding the current to an electrode in an electrochemical cell. This can be modelled using reaction convection diffusion equations, the current being a linear functional of their solution. Boundary singularities at the edge of the electrode cause difficulties when solving these problems using standard numerical techniques due to a slow rate of convergence, thus an alternative method is needed. We present an adaptive finite element algorithm in which an a posteriori error bound is derived for a numerical approximation of the current for a simple problem. This error bound is used to refine the mesh where necessary until the estimated error is within a prescribed tolerance. This method has the advantage of being more efficient than standard techniques and the error bound guarantees the accuracy of the solution. We conclude by discussing results for more complicated problems and illustrating that these compare very favourably with previous results obtained using standard numerical techniques.

Preconditioning eigenproblems arising from discretizations of stiff parameter dependent semilinear PDEs

Stuart C. Hawkins¹ & Alastair Spence

¹University of Bath

The eigenvalues of preconditioned Jacobians may be easier to compute than those of the Jacobian itself but can we use them to detect bifurcation points? For some stiff parameter dependent semilinear PDEs there is a natural preconditioner available, but with this preconditioner the eigenvalues are transformed in a complicated way which we cannot analytically invert. We present two methods which use the eigenvalues of

this preconditioned Jacobian to detect a Hopf bifurcation. We illustrate these methods by applying them to the Tubular Reactor problem.

Uniformly accurate numerical solution of singular perturbation problems with parabolic boundary layers.

Alan Hegarty¹, Paul A. Farrell, John J.H. Miller, Eugene O'Riordan & G.I. Shishkin

¹University of Limerick

Parabolic boundary layers arise, for example, in the solutions of problems involving laminar and turbulent fluid flows near walls. Their structure controlled by the properties of the fluid and the nature of the flow and, in particular, by whether the relevant boundary condition is slip nor no slip. The errors in the numerical solutions of these problems obtained using traditional numerical methods are extremely large, especially when approximation to derivatives of the solution are required; for example, when effects related to drag, flux or separation/attachment have to be computed. For a model class of linear problems, whose solutions have boundary layers of the above character, we examine numerical methods, based on upwind finite difference operators and piecewise-uniform fitted meshes, for computing the solutions and derivatives.

Adaptive Error Control in Solving Ordinary Differential Equations by the Discontinuous Galerkin Method

V. Heuveline¹ & R. Rannacher

¹University of Heidelberg

The conventional adaptive step-size strategies for solving ordinary differential equations by difference methods are based on a priori error estimates in terms of local truncation error. Unlike these approaches, the Galerkin methods for ordinary differential equations allow to consider time-stepping scheme based on a posteriori error estimators. These techniques which are well known in the context of partial differential equations, are based on the Galerkin orthogonality inherent to such schemes. A duality argument results in asymptotically optimal weighted a posteriori error estimates.

We consider these methods with arbitrary order and propose an analysis with special emphasize on existence/nonexistence of explicit schemes as well as a detailed description considering Lagrange polynomials associated with Radau or Lobatto quadrature abscissas for the shape and test functions. This approach is developed here for non-stiff initial value problem and is illustrated by several test problems.

Numerical Stability for Stochastic ODEs

D. J. Higham

University of Strathclyde

I will consider the linear stability of numerical methods for stochastic ordinary differential equations (SDEs). The focus will be on mean-square stability of two methods that reduce to the Theta Method on deterministic problems. I will approach the topic from the viewpoint of a traditional numerical analyst, and investigate whether the methods generalise the deterministic A-stability property. No background knowledge in SDEs will be assumed.

A Block Algorithm for Matrix 1-Norm Estimation, with an Application to 1-Norm Pseudospectra

Nicholas J. Higham¹ & Françoise Tisseur

¹University of Manchester

The matrix 1-norm estimation algorithm used in LAPACK and various other software libraries and packages has proved to be a valuable tool. However, it has the limitations that it offers the user no control over the accuracy and reliability of the estimate and that it is based on level 2 BLAS operations. A block generalization of the 1-norm power method underlying the estimator is derived here and developed into a practical algorithm applicable to both real and complex matrices. The algorithm works with $n \times t$ matrices, where t is a parameter. For $t = 1$ the original algorithm is recovered, but with two improvements (one for real matrices and one for complex matrices). The accuracy and reliability of the estimates generally increases with t and the computational kernels are level 3 BLAS operations for $t > 1$. The last $t-1$ columns of the starting matrix are randomly chosen, giving the algorithm a statistical flavour. As a by-product of our investigations we identify a matrix for which the 1-norm power method takes the maximum number of iterations. As an application of the new estimator we show how it can be used to efficiently approximate 1-norm pseudospectra.

Higher Order Approximation of Inertial Manifolds

Adrian Hill¹ & M.A. Falcon

¹University of Bath

The Inertial Manifold of a nonlinear dissipative PDE is characterised as a finite-dimensional subset of phase space onto which all trajectories converge with exponential speed. This talk reviews the very important paper of Jones, Stuart and Titi on the approximation of the Inertial Manifold and considers the new question of higher-order convergence. A pseudospectral-trapezoidal approximation of the Kuramoto-Sivashinsky equation is considered as an example.

The 'enriched' hybrid Galerkin method

Robert A. Horrocks¹, Ivan G. Graham & Stefan A. Sauter

¹University of Bath

In the practical implementation of the boundary element method in 3D the formation of the stiffness matrix often forms a dominant part of the computation time. For N degrees of freedom the cost of assembling the complete matrix is CN^2 , with C moderately large and dependent on the number of kernel evaluations used by the integration routine.

In previous work by Graham, Hackbusch and Sauter a new fast quadrature method for approximating the stiffness matrix was introduced. For example, in the case of piecewise linear basis functions on a mesh with N nodes, and under general assumptions, the simplest version of the method computes the matrix using $N^2 + O(N^\gamma)$ kernel evaluations, for some $\gamma < 2$ as $N \rightarrow \infty$. The N^2 term comes from the fact that most of the matrix is computed using novel quadrature rules which just use kernel evaluations at pairs of nodes, with the lower order part coming from conventional rules applied to the small remaining part of the matrix.

In this talk we briefly review this 'hybrid' method and introduce a variant which, as well as using kernel evaluations at nodes of the mesh, uses additional evaluations at some of the centroids of the triangles. This method, which we call the 'enriched' hybrid method, has a slightly higher complexity than the hybrid method, but has the advantage that for moderate N it may be used to compute more elements of the matrix.

We illustrate the method with some numerical experiments on a Dirichlet screen problem for Laplace's equation.

hp-Adaptive Finite Element Methods for First-Order Hyperbolic Problems

Paul Houston¹, E. Süli & Ch. Schwab

¹Oxford University Computing Laboratory

We consider the *a posteriori* error analysis of hp-discontinuous Galerkin finite element approximations to first-order hyperbolic problems. In particular, we discuss the question of error estimation for linear functionals, such as the outflow flux and the local average of the solution. Based on our *a posteriori* error bound we design and implement the corresponding adaptive algorithm to ensure reliable and efficient control of the error in the prescribed functional to within a given tolerance. This involves exploiting both local polynomial enrichment and local mesh subdivision. The theoretical results are illustrated by a series of numerical experiments.

[1] P. Houston, R. Rannacher, and E. Süli. *A posteriori error analysis for stabilised finite element approximations of transport problems*. Oxford University Computing Laboratory Technical Report NA-99/04, 1999 (submitted for publication).

[2] P. Houston, Ch. Schwab, and E. Süli. *Stabilised hp-finite element methods for first-order hyperbolic problems*. Oxford University Computing Laboratory Technical Report NA-98/14, 1998. (submitted for publication).

Dynamics of Variable Time-Stepping Numerical Methods

A. R. Humphries

Sussex University

Adaptive solvers are used increasingly in applications to simulate nonlinear dynamics. The "standard" variable time-stepping algorithm tries to control the local error, based on a heuristic argument valid for small h . However, this algorithm can result in step-sizes which are of $O(1)$ for which the local error is not well-controlled.

Moreover, in chaotic attractors, the flow on the attractor is often organised by the unstable manifolds of the fixed points, and it is thus necessary to be able to obtain good numerical approximations in the neighbourhood of a fixed point. In such a neighbourhood there will be orbits which are unbounded in time but bounded in phase space, and error control in time is bound to fail.

In this talk we use phase space techniques to present some of the problems that arise with standard variable time-stepping methods applied to dynamical systems, and investigate possible improvements.

BDF2 blends for convection dominated flows

Willem Hundsdorfer

CWI

In this talk several blends of implicit and explicit time integration schemes are considered, based on the well-known BDF2 method. The schemes are applied to convection-diffusion problems with dominating convection. A fully implicit treatment of convection terms is often not very efficient. We shall deal with schemes that are implicit in the convection terms only locally in space, in those regions where the Courant numbers are large, without introducing the internal inconsistencies that are common with many time-splitting methods. Along with implementation aspects of the implicit relations, we shall discuss accuracy of the schemes, positivity and monotonicity properties.

Numerical solution of the critical flow on a rotating cylinder

Roland Hunt

Strathclyde University

In order to spread bread with runny honey, it is necessary to rotate a knife dextrously as honey is taken from the pot. In the same way it possible for a viscous liquid to remain attached to a rotating cylinder. The resulting steady free boundary problem can be easily solved numerically by first mapping to domain onto a rectangle, discretising the equations pseudospectrally and using Newton's iteration to solve ensuing algebraic system. Interest lies in ascertaining the maximum amount of liquid that can be sustained on the cylinder for a specified angular velocity and in particular confirming an asymptotic expansion when the fluid thickness is thin. Using various numerical techniques it is possible to find the critical amount and to confirm the series. However an analysis of the numerical solution reveals that the expansion is very limited and suggests a better alternative expansion.

Updating a correlation matrix by making use of hyperbolic transformations

D. Janovska¹ & Gerhard Opfer

¹Prague Institute of Chemical Technology

A computational method for singular values of an updated correlation matrix will be presented. The main advantage of the algorithm consists in the fact that a triangularization of an old data matrix is used. The method is based on hyperbolic Givens and hyperbolic Householder transformations. Main properties of the transformation matrices will be given. Stability of the method will be discussed.

An Optimal Domain Decomposition Preconditioner

P. K. Jimack¹, R. E. Bank & S. V. Nepomnyaschikh

¹University of Leeds

This presentation will introduce a new domain decomposition preconditioner which is ideally suited for use in a parallel adaptive finite algorithm for the solution of self-adjoint partial differential equations. The preconditioner is based upon the overlapping additive Schwartz algorithm but has the novel feature that the subspace decomposition corresponds to an overlap of just a single element of each mesh in a sequence of hierarchically refinement meshes. Unlike conventional overlapping additive Schwartz methods which require $O(h^{-2})$ fine mesh elements in the overlap regions in order to be optimal (i.e. to have yield a preconditioned system whose condition number is independent of h , the fine mesh size, and H , the coarse mesh size), this hierarchical technique may be proved to be optimal with just $O(h^{-1} \log h^{-1})$ elements in the overlap regions. Furthermore, the use of a sequences of hierarchically refined meshes within the algorithm allows it to be naturally applied to the adaptive solution of differential equations based upon local h -refinement. As well as providing an overview of the algorithm and an outline of the optimality proof the talk will also include a description of a small number of numerical experiments which verify that the preconditioner is indeed optimal and that it is far more computationally efficient than using the conventional overlap width, which is independent of the level of refinement in the mesh. If time permits extensions to nonlinear and non-self-adjoint problems will also be discussed.

The Box Scheme for Transcritical Flow

Thomas C. Johnson¹, P. K. Sweby & M. J. Baines¹University of Reading

The Preissmann box scheme is widely used in the modelling of river hydraulics. This implicit four point scheme readily permits non-uniform spacial grids and does not suffer any CFL restriction on the maximum allowable time step. The resulting system of discrete equations is block-bidiagonal and therefore inversion is relatively cheap compared to many other implicit schemes. Its main failing however is that it cannot accurately model transcritical flow. A modification to the scheme to circumvent this problem was introduced in (Morton et al. J. Comp. Phys., 114:209-226, 1994), and applied to the steady Euler equations. In this talk the technique is applied to transcritical non-steady shallow water flow.

Accuracy in solving multivariate polynomials using Macaulay resultants**Gudbjorn F. Jonsson¹ & Stephen Vavasis**¹Cornell University

Solving polynomials and systems of polynomial equations is a fundamental problem for geometric modeling and arises in applications such as mesh generation and graphics. The problem of finding the roots of a univariate polynomial can be converted into an eigenvalue problem via the companion matrix. The same can be done for a system of multivariate polynomials using the algebraic concepts of u-resultants and Macaulay resultant matrices. We will show how these matrices are constructed and propose numerical techniques to stabilize this method of solving a system of polynomial equations.

Green's tensors for preconditioning steady-state Navier-Stokes equations: Part II - Application**David Kay¹ & Daniel Loghin**¹Oxford University

An efficient method for solving the sparse linear system of equations arising from the finite element or finite difference discretisations of the linearised steady state Navier-Stokes or Oseen equations is given.

Due to features such as boundary layers in the true solution of these equations, it may be necessary to reduce the element size in proportion to any decrease in viscosity. Furthermore, the use of Krylov subspace iterative methods to solve such systems produces convergence rates that are dependent on both element size and viscosity. Hence, a preconditioner that has little or no dependence on either mesh size or viscosity is required. A practical and efficient implementation of such a preconditioner arising from the consideration of the continuous inverse is shown.

Simple multigrid cycles and preconditioned conjugate gradient iterations are used to give an inexact solve on the preconditioner. Convergence rates are seen similar to those using exact inversion of the preconditioner. That is, only mild dependence on the viscosity parameter and no dependence on the mesh size.

Constraint Preconditioning for Indefinite Linear Systems**Carsten Keller¹, Andy Wathen & Nick Gould**¹University of Oxford

The problem of finding good preconditioners for the numerical solution of indefinite linear systems of a sort which arise in areas such as constrained optimization, least-squares problems, structural analysis and also saddle point problems is considered. In this context, the coefficient matrix of the linear system $Ax = b$ takes the special form

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

where H is an $n \times n$ symmetric matrix block and B is a $m \times n$ block which has full rank m . We assume throughout that $m \leq n$.

In deriving an efficient preconditioner theory for the above system, we put special emphasis on preconditioners that have the same 2×2 block structure as A , and which incorporate the original (1,2) and (2,1) blocks. In constrained optimization, as well as many other areas, these blocks are usually associated with constraints.

We give analytic results concerning the spectrum and form of the eigenvectors of the preconditioned matrix and its minimum polynomial. The consequences of these results are considered for a variety of Krylov subspace methods and also for the sparse direct solver MA27 of the Harwell Subroutine Library. In particular, to show the favourable aspects of the above preconditioner, it makes sense to compare unpreconditioned with preconditioned strategies. The indefinite nature of A suggests the use of the minimum residual method of Paige and Saunders in the unpreconditioned case. We apply two slightly different strategies in order to implement the preconditioner. The first method applies the standard (full) generalised minimum residual method of Saad and Schultz, which is mathematically equivalent to the minimum residual method in case of symmetric coefficient matrices. The second method applies a conjugate gradient like algorithm that was first proposed by Gould, Hribar and Nocedal. Their algorithm is based on the idea of computing an implicit basis Z that spans the nullspace of B , and which is consequently used to remove the constraints from the system of equations, thus allowing the application of the conjugate gradients method to the (positive definite) reduced system. Finally, we compare the three Krylov subspace based methods with the direct solver MA27 of Duff and Reid, and show that, for large systems, Gould et al.'s method can still bring considerable improvements even when MA27 fails due to the dimension of the coefficient matrix A .

A shooting method for the generation of the best L_1 piecewise linear interpolation

R. Ketzscher¹ & S. A. Forth

¹Cranfield University

An algorithm for the direct generation of the best L_1 piecewise linear interpolation of real-valued functions is derived. A geometric interpretation of the optimality conditions for three adjacent points (knots) allows us to develop a shooting method. In this a nonlinear 3 term recurrence relation is solved to successively determine one point's location based on two preceding ones. For a given interval, the method starts at the left and the first interior knot point is selected and consequently adjusted in order that the shooting method produces the correct end point at the right of the interval.

The information used, the quality of the resulting grids and the efficiency of the algorithm are compared with other methods, such as equidistribution. It is shown that even without using higher order derivatives and quadrature, grids are generated for which the global error is minimised, as opposed to just equidistributed. The downside of the suggested implementation is that to ensure robustness the utilised optimisation routines are slower than comparable equidistribution methods.

Newton's Method for Solving a Quadratic Matrix Equation

Hyun-Min Kim¹ & Nicholas J. Higham

¹University of Manchester

We show how to incorporate exact line searches into Newton's method for solving the quadratic matrix equation $AX^2 + BX + C = 0$, where A , B and C are square matrices. The line searches are relatively inexpensive and improve the global convergence properties of Newton's method in theory and in practice. We also derive a condition number for the problem and show how to compute the backward error of an approximate solution.

Homoclinic Shadowing

Huseyin Kocak¹, B. Coomes & K. Palmer

¹University of Miami

Homoclinic points play a central role in chaotic dynamical systems where numerical computations are inherently dangerous. Using the techniques of shadowing, we present a general numerical method for proving the existence of homoclinic points in specific dynamical systems. We demonstrate the effectiveness of our method on several famous examples of chaotic dynamical systems.

The Convergence of Shooting Methods for Singular Boundary Value Problems

Othmar Koch¹ & Ewa B. Weinmueller

¹Vienna University of Technology

We consider singular boundary value problems (BVPs) of the form

$$\begin{aligned} z'(t) &= \frac{M(t)}{t} z(t) + f(t, z(t)), \quad t \in (0, 1], \\ M(0)z(0) &= 0, \\ g(z(0), z(1)) &= 0, \end{aligned}$$

where f and g are smooth functions and g is chosen such that the BVP is well-posed. In order to solve the BVP we apply single and parallel shooting to reduce the problem to a set of initial value problems (IVPs) which are integrated from left to right.

Convergence properties of the solution of the boundary value problem are investigated under the assumption that a numerical method for IVPs with a level of accuracy of $O(h^p)$ is used.

For these considerations we have to use some nonstandard techniques to show that the shooting method is well-defined for well-posed singular BVPs, prove perturbation results for singular IVPs and the smooth dependence on parameters for the IVPs, which does not follow from classical theory. Finally, a convergence result for the perturbed Newton iteration, which occurs in the solution process of the sets of nonlinear algebraic equations involved, is given.

Structural Optimization with Stability Constraints: Solving Nonconvex Semidefinite Programs

M. Kocvara¹ & F. Jarre¹University of Erlangen

Structural optimization seeks to find the best design of mechanical structures under given loads. Standard approaches try to minimize the volume/weight of the structure such that the structural stresses are kept within technically feasible bounds. Typically, such models lead to high-dimensional nonlinear programs. There is a serious limitation, though. These models do not count with possible instability of the structure. Real life experience has shown that in some cases the structures like bridges or aircrafts may fail not on account of high stresses but due to insufficient elastic stability.

We will present an optimization problem targeting at the same goals as the standard models, but adding a constraint on the elastic stability of the optimal structure as well. This is a mathematical program with a linear objective function and a constraint on positive semidefiniteness of certain matrix which depends on the design variable in a nonconvex way. We propose a solution method that applies to general nonconvex semidefinite programs. The method combines ideas of a predictor-corrector interior-point method, of the SQP method, and of trust region methods. The outer structure of our algorithm is given by the interior-point method. The linear systems of the Newton step and of the predictor step are replaced by quadratically constrained quadratic programs; these are of a special structure and can be solved directly.

Numerical examples will demonstrate the behaviour of the new method.

The Application of Multiple Shooting to Singular Boundary Value Problems**Peter Kofler¹ & Winfried Auzinger**¹Vienna University of Technology

Multiple shooting is a standard technique for the numerical solution of boundary value problems. We discuss the application of multiple shooting techniques to a certain class of nonlinear singular boundary value problems. Particular attention is paid to the methodology for the integration of the underlying initial value problems. To this end we use the implicit Euler scheme, serving as a basic method for the acceleration technique known as Iterated Defect Correction. This yields a stable initial value integrator realizing a high order approximation for the singular case (a nontrivial result). Simple shooting based on this integration method performs successfully, and the extension to multiple shooting is straightforward. A number of experimental results illustrating this approach are presented.

The dynamics of adaptive timestepping ODE solvers**Harbir Lamba**

George Mason University

A framework is described for adaptive timestepping algorithms which is general enough to include many of the timestep selection mechanisms currently used. For this class of algorithms the finite-time convergence properties are found to be independent of the timestep selection mechanism, depending only upon the precise form of the local error estimate. This framework also facilitates the analysis of such algorithms as dynamical systems and their asymptotic convergence and stability properties.

On certain bivariate local spline quasi-interpolating operators**Paola Lamberti¹ & Catterina Dagnino**

¹University of Turin

We investigate some quasi-interpolating operators defined by a B-spline basis in the bivariate spline space $S_2^1(\Delta_{mn}^{(2)})$ (i.e. the space of bivariate splines of total degree 2 and smoothness 1 with respect to the partition $\Delta_{mn}^{(2)}$, obtained by partitioning a rectangular domain D into uniform subrectangles and adding to each one both diagonals) ([1]).

Such approximation schemes have several interesting applications both in surfaces modelling and in the numerical solution of engineering problems ([2,3]).

For the above operators we present new convergence results with particular reference to the approximation order and we give error bounds.

[1] C.K. Chui and R.-H. Wang, *On a bivariate B-spline basis*, Scientia Sinica **XXVII** (1984), 1129-1142.

[2] C. Dagnino and P. Lamberti, *Numerical integration of 2-D integrals based on local bivariate C^1 quasi-interpolating splines*, Adv. Comp. Math. **8** (1998), 19-31.

[3] R.-H. Wang and You Lu, *Quasi-interpolating operators and their applications in Hypersingular integrals*, J. Comp. Math. **16** n.4 (1998), 337-344.

Boundary integral methods for singularly perturbed boundary value problems

S. Langdon¹ & I. G. Graham

¹Durham University

We consider boundary integral methods applied to boundary-value problems for the positive definite Helmholtz-type problem

$$-\Delta U + \alpha^2 U = 0$$

in a bounded or unbounded two-dimensional domain, with the parameter α real and possibly large. Applications arise in the implementation of space-time boundary integral methods for the heat equation, where α is proportional to $1/\sqrt{\delta t}$, and δt is the time step. The corresponding layer potentials arising from this problem depend nonlinearly on the parameter α and have kernels which become highly peaked as $\alpha \rightarrow \infty$, causing standard discretisation schemes to fail. Here we propose a new collocation method with an error estimate that is independent of α , and we present numerical experiments on a model problem demonstrating the robust convergence rate as $\alpha \rightarrow \infty$.

Discrete Least Squares for Hyperbolic Equations and Systems Incorporating Mesh Movement

S. J. Leary¹, M. J. Baines & M .E. Hubbard

¹University of Reading

A finite volume method is presented for steady advection equations and conservation laws on unstructured meshes incorporating mesh movement. The method can substantially improve the resolution of sharp features (contacts, shocks) by solving on an optimal mesh. Results are presented for a number of steady state test problems, including scalar advection and the shallow water equations in 2-D.

A great deal of effort is currently being put into mesh refinement near shocks using mesh subdivision, but similar improvements in resolution can also be obtained much more cheaply by minor adjustments to the

mesh. A requirement is a criterion for mesh adjustment, paralleling the monitor functions used in mesh subdivision.

We consider a descent approach using a least squares measure of the residual. The procedure is to interleave mesh adjustment steps between steps of a least squares type scheme. For scalar equations there is a close relationship with the method of characteristics. For systems of equations additional linearisation is necessary to make progress: however, encouraging results are obtained for flows in channels governed by the shallow water equations. A discontinuous least squares method for shocked flows is described which uses the nonlinear shock jump residual to adjust the mesh.

Singular differential equations in fluid flow

A. C. Lemos¹, M. J. Baines & N. K. Nichols

¹University of Reading

Many physical phenomena are described by systems of conservation laws, for example the Shallow Water Equations and the Euler Equations of compressible gas dynamics. These systems of equations are nonlinear and hyperbolic in nature, admitting discontinuous solutions. In the steady case both the Shallow Water Equations and the isentropic Euler equations for gas flow can be reduced to a single nonlinear differential equation with singular coefficients (because the continuity equation can be integrated and becomes algebraic). It has been shown that the upwind Engquist-Osher scheme applied to the reduced problem can provide approximations which not only deal with singularities but also provide a consistent treatment of boundary conditions, since the scheme respects the direction of the flow. We describe this use of the Engquist-Osher scheme and speculate on the method as a way of solving the full Euler Equations.

A quadratic-bundle-based decomposition for stochastic QP

Sven Leyffer¹, Jeff Linderot & Steve Wright

¹University of Dundee

We consider stochastic Quadratic Programs arising for instance in financial applications such as the determination of efficient portfolios.

We propose a quadratic-bundle-based decomposition scheme for solving stochastic QP. Unlike traditional approaches, we generate second order cuts and use these cuts in a bundle-based decomposition scheme. Finite convergence of the resulting algorithm is established.

Computational experience with the new algorithm is presented.

Uniform Superconvergence of a Galerkin Finite Element Method on Layer-Adapted Meshes

Torsten Linß

Technische Universität Dresden

We consider a Galerkin finite element method that uses piecewise bilinears on a class of Shishkin-type meshes for a model singularly perturbed convection-diffusion problem on the unit square. The method is shown to be convergent, uniformly in the diffusion parameter, of almost second order in a discrete weighted energy norm. As a corollary we derive global L^2 and local pointwise error estimates.

Green's Tensors for Preconditioning the Steady-State Navier-Stokes Equations: Part I - Theory

Daniel Loghin¹ & David Kay

¹Oxford University Computing Laboratory

In this paper we introduce efficient preconditioners for problems arising from mixed finite element formulations. Our approach makes recourse to the Green's tensor, which, as the continuous inverse, holds the answer to efficient preconditioning. Our efforts focus on the appropriate choice of discrete inverse based on the continuous one. In the case of the Stokes/Navier-Stokes equations this problem reduces to finding a good approximation to the Schur complement of the system matrix. The Green's tensor technique yields a simple factorisation of the Schur complement with a nearly optimal performance: mild dependence on the viscosity parameter and reducing number of iterations with decreasing mesh size. The latter feature is common for preconditioners based on continuous inverses.

Quadrature rules for the hypercube of optimum trigonometric degree

James Lyness

Argonne National Laboratory

Theory and results about optimum rules of polynomial degree for the hypercube have been treated at length in the literature. The corresponding theory and results for rules of trigonometrical degree is not well known. In this talk, I describe briefly a few of the salient features of this theory.

This work was supported by the Office of Scientific Computing, U.S. Department of Energy, under Contract W-31-109-Eng-38.

A moving finite element method for two-dimensional Stefan problems

J. A. Mackenzie¹ & M. L. Robertson

¹Strathclyde University

In this talk we consider the development of an r-adaptive finite element method for two-dimensional Stefan problems. The moving grid nodes evolve according to a gradient flow equation of the functional

$$I(\xi) = \frac{1}{2} \int_{\Omega} [(\nabla \xi)^T G^{-1} \nabla \xi + (\nabla \eta)^T G^{-1} \nabla \eta] dx,$$

where $\xi(\mathbf{x}) = (\xi, \eta)$ is a one-to-one mapping of the physical to the computational domain and G is a 2×2 SPD monitor matrix. Various choices of G will be considered and tested on a solidification problem.

On the numerical recovery of a holomorphic mapping from a finite set of approximate values

J. M. Marban¹ & C. Palencia

¹University of Valladolid, Spain

The least-squares method for the recovery of a holomorphic mapping from given perturbed nodal values is reconsidered. The mapping is assumed to be a priori bounded by a known quantity, so that the recovery problem is well-posed. The numerical algorithm deals the a priori bound as a constraint. The present analysis shows that for nodes that are the zeroes of Jacobi polynomials a quasioptimal algorithm results with a fairly moderate number of nodes. The analysis also takes into account the effect of the numerical linear algebra involved. Some numerical experiments are presented.

Using data assimilation to estimate systematic model error

M. J. Martin¹, N. K. Nichols & M. J. Bell

¹University of Reading

Data assimilation is a method for estimating the state of a system by combining observational data with a prior estimate of the state, usually

obtained from a numerical model. There are two main types of data assimilation: sequential (3D) methods, which will be discussed here, and

4D methods. In the derivation of these methods, it is assumed that model error is uncorrelated in time which, in practice, is rarely the case. To account for time correlated model error, a vector of model error variables is appended to the state vector and this augmented state is then treated

using the same data assimilation methods as before. A priori knowledge of the model error evolution is needed to close the problem and some examples of how this might be specified are discussed.

The method of state augmentation to estimate model error is applied to two test problems using the Optimal Interpolation data assimilation method. The Lorenz equations, a system of nonlinear ordinary differential equations, are given model error in the form of a constant forcing. It is shown that this error can be estimated by using a constant model for the model error evolution. The heat equation, a simple partial differential equation, is used to test whether incorrect boundary conditions can be taken into account in the same way.

Convergence Analysis of the Discrete QR Method for Computing Lyapunov Exponents

Edward McDonald¹ & Des Higham

¹University of Strathclyde

The discrete QR method is a popular technique for approximating Lyapunov exponents, yet there is little convergence theory to justify its use. In this talk we consider a constant coefficient linear dynamical system, where the Lyapunov exponents reduce to the real parts of the Jacobian eigenvalues. In this case the algorithm is closely related to the QR iteration for computing eigenvalues. Using a result about Schur vector convergence in the QR iteration we establish sharp convergence rates for the Lyapunov exponents in the discrete QR method. Although derived on a simple test problem, the convergence analysis suggests a practical approach for balancing the errors that arise from (a) discretising in time and (b) truncating an infinite integral.

The rational Lanczos method for the Hermitian eigenvalue problem

Karl Meerbergen

Rutherford Appleton Laboratory

Applications such as the modal analysis of structures and acoustic cavities require a number of eigenvalues and eigenvectors of large scale Hermitian eigenvalue problems. The most popular method is probably the spectral transformation Lanczos method. An important disadvantage of this method is that a change of pole requires a complete restart. In this talk, we investigate the use of the rational Krylov method for this application. This method does not require a complete restart after a change of pole. We prove that for a specific implementation, numerical instabilities can occur when the pole is not chosen carefully. Numerical examples illustrate the theory.

Integral Equation Methods for Scattering by Rough Surfaces

Anja Meier¹ & Simon N. Chandler-Wilde

¹Dept. of Maths & Stats, Brunel University

We consider the problem of wave scattering by infinite one-dimensional rough surfaces. As a fundamental solution in the integral equation formulation either the free-field Green's function (which is the standard approach) or a half-space Green's is used. The integral equation is discretized using the Nyström method described in the talk by T. Arens. Then an iterative scheme in which the kernel is approximated by Taylor or Chebychev series expansions is used. We will present a stability result and show some numerical results including a comparison with the diffraction grating results in the talk of T. Arens.

A spectral method for computing viscoelastic flows

Sha Meng

De Montfort University

A spectral element method for computing viscoelastic flows is presented. The spectral element methods are high-order weighted residual techniques for the approximation of partial differential equations that combine the generality of finite element methods with the accuracy of spectral methods. In the spectral element discretization, the computational domain is broken into a series of elements, the velocities and pressure in each element are represented as high-order Lagrangian interpolant through Gauss-Legendre Lobatto points, respectively. The weak formulations of the viscoelastic flows in two space dimensions are also discretized with spectral element approximation and Gauss-Lobatto-Legendre quadratures. The Uzawa algorithm is applied to decouple the velocities from the pressure. The equations that result for the pressure and the velocities are solved by preconditioned conjugate gradient iteration. The numerical solutions are investigated on the Stokes problem and the contraction flow benchmark problem with upper-convected Maxwell (UCM) model.

On finite-difference methods for elliptic problems with discontinuous coefficients and jumps

Mathias Moog

ITWM, University of Kaiserslautern

The equation $(k u_x)_x = f$ for two phase potential flow in 1D is considered, with a jump in the potential u on the interface and continuous fluxes $k u_x$ across the interface.

Different finite difference discretisations of this problem are proposed in literature. A straightforward way is to smear out the jumps and use standard finite difference approximations. Other approaches are for example the immersed interface method of Leveque and Li [SIAM J. Numer. Anal. 31, No.4, 1019-1044 (1994)] or

the explicit jump immersed interface method of Wiegmann. They modify the finite difference approximation near interface to resolve the jumps.

In the case of a zero right hand side and piecewise constant k the different discretisations are compared. For three point stencils they all lead to the same discrete equations.

To establish the connection between the different methods the 'discrete moment condition' of Beyer and Leveque [SIAM J. Numer. Anal. 29, No.2, 332-364 (1992)] is used. This condition was originally used to define a discrete δ function. It will be extended to handle the derivative of a discrete δ function as well.

Laguerre approximation of stable manifolds

Gerald Moore

Imperial College

The computation of a point on the stable manifold of a stationary solution for an autonomous system of ODE's leads to an equation posed over an infinite interval. Standard approximation methods therefore usually involve truncation or a change of independent variable. In this talk we suggest an alternative approach based on Laguerre polynomials. We also show how this leads to a spectral method for approximating connecting orbits.

Cheap Global Error Estimation of Explicit Runge-Kutta Methods

Ander Murua¹ & Joseba Makazaga

¹University of the Basque Country

We propose a class of one-step integrators for ODEs that provide an estimation of the global error along with the numerical solution. The schemes that we propose can be considered as a generalization of the globally embedded RK methods of Dormand, Gilmore and Prince (1994). A few schemes that we have constructed based on optimized standard RK methods are presented.

We report numerical experiments testing the performance of the schemes in variable step-size implementation. The numerical results seem to indicate that our method gives useful information on the behaviour of the global error while being nearly as efficient as the underlying standard RK scheme.

The Effect of Roundoff Error on the Numerical Solution of a Problem with Boundary Layers

A. Musgrave¹, J.J.H. Miller, E. O'Riordan & G.I. Shishkin

¹Trinity College

We consider a reaction-diffusion problem on the unit interval $[0,1]$ in which the highest order derivative is multiplied by a small parameter ε . The parameter ε is proportional to the diffusion coefficient and when ε is small two boundary layers typically exist in the solution. It has been shown theoretically that the standard second order centered finite difference operator on a piecewise uniform fitted mesh gives numerical solutions that converge uniformly in the maximum norm for all values of ε in the range $0 < \varepsilon \leq 1$ to the exact solution of this problem. However numerical results calculated using double precision arithmetic appear to indicate a failure of the numerical solutions to converge. Detailed investigations using quadruple precision arithmetic on the QUB/TCD IBM SP2 show that this lack of convergence is due to the presence of roundoff error which in some cases is larger in magnitude than the discretisation error. The convergence rate of the numerical

method is determined experimentally in quadruple precision arithmetic and is found to agree with the theoretical estimates.

Structured Perturbations and Robust Eigenstructure Assignment in Quadratic Matrix Pencils

N. K. Nichols¹ & J. Kautsky

¹University of Reading

We aim to construct a state feedback control to ensure that a given system of n second-order linear differential equations has a specified set of $2n$ eigenvalues and that the eigenvalues are as insensitive as possible to perturbations in the system coefficients. Second-order systems can be written in first-order form and then known methods for eigenstructure assignment can be applied to determine the required feedback. This approach does not take advantage of the special eigenstructure of the original quadratic matrix pencil, however, nor does it take into account the structure of the allowable perturbations of the system. Here we derive robustness measures for the eigenvalues of the quadratic pencil and show that equivalent measures can be obtained for the linear form of the system subject to structured perturbations. We describe a procedure for assigning eigenvalues to the linear form that are robust with respect to the structured perturbations and that take advantage of the special properties of the eigenstructure of the system.

A new fitting for a spectral approach

F Z Nouri

University of Annaba

We propose to solve the Navier-Stokes problem by a spectral method. A new procedure, based on the "joint method" is considered. First, we solve the axisymmetric Stokes problem and then the 3D Navier-Stokes equations. We make use of the Glowinski technique (Numerical Methods for Variational Problems, Springer Verlag, 1982) combined with a sub-domain method without recovery.

A spectral element method for the Navier-Stokes equations with improved accuracy

Julia Novo¹ & Javier de Frutos

¹Universidad de Valladolid

We present a procedure to enhance the accuracy of spectral element methods for the evolutionary Navier-Stokes equations. The approximations to the velocity and the pressure obtained using a spectral element method are postprocessed by solving a discrete Stokes problem only once, when the time evolution is completed. The analysis shows that this procedure improves the order of convergence both for the approximations to the velocity and the pressure. The choice of a discrete pressure space endowed with an inf-sup condition independent of the discretization parameter leads to optimal error bounds for the pressure.

On some problems with the hyperbolic Givens transformation

Gerhard Opfer

University of Hamburg

If a square matrix $\mathbf{A}$ with real or complex elements is orthogonal, then by definition $\mathbf{A}^H \mathbf{A} = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix. There are some applications (e. g. updating of a matrix in certain contexts, see Golub & Van Loan's book, last chapter) where a transformation of the form (*) $\mathbf{A}^H \Phi \mathbf{A} = \Phi$ is required, where Φ is a given diagonal matrix with diagonal entries ± 1 .

The terminology is not quite unique. Some authors call a matrix $\mathbf{A}$ with (*) *hypernormal with respect to Φ* . Let us also use this notation. The problem is, how to transform a given matrix into a such a hypernormal matrix. It turns out, that Householder's transformation can be put into a hyperbolic Householder transformation, but for Givens' transformation, there are some obstacles, and the general question is, how to tailor a hyperbolic Givens rotation.

This will be the topic of the lecture.

Geometric theory of fully nonlinear parabolic equations under discretization

Alexander Ostermann

Universität Innsbruck

The qualitative behaviour of Runge-Kutta time discretizations of fully nonlinear parabolic problems is discussed. In particular, it is shown that the discretization preserves the geometric properties of the underlying problem in a neighbourhood of a hyperbolic equilibrium point. The analysis is based on analytic semigroups and makes use of the Hölder continuity of the solution.

Reference: C. González, A. Ostermann, C. Palencia, and M. Thalhammer: *Runge-Kutta time discretization of nonlinear parabolic problems near equilibria*, in preparation.

Coupled Waves Method of Analysing Boundary Conditions

M. Parsaei

Tehran University

When solving conservation laws numerically the best method for analysing boundary conditions and reflections at the boundaries is the time fourier transform (t-fourier transform). This enables us to study the the inter-relation between the amplitude of the solution wave at neighbouring nodes in x-direction. The usual space fourier transform (x-fourier transform) is unsuitable for propagation phenomena due to the inter-action between waves of different wave lengths. It is possible to merge these two methods by assuming that the solution wave is the result of a coupling between groups of independent waves. By decoupling these wave the x-fourier transform can be used on each. The inter-relation between these waves is governed by the approximating difference equation. In this talk we use this method to study the behaviour of the outflow boundary conditions and some numerical results are presented.

Feature of the stress state determination of viscoelastic composites

Boris E. Pobedria

The Moscow State University

The determination of a stress-strain state in viscoelastic composites is very difficult problem. Therefore it is necessary to search for the traditional approaches.

1. As a rule, the constitutive relations connecting stresses and strains are nonlinear integrated operators on time. Their representation as a sum of integrals of a growing multiplicity requires the experimental definition of the large number of creep and relaxation functions.

If the nonlinearity is described by single integrals, some experiments (for example, on cyclical loads) can not be explained. We offer functional relations, which allow to find experimentally all material functions and to take into account effects explained only by the theory with multiple integrated operators.

2. Frequently diameter of the structure element of a composite is on 5-7 ordinal less size of a body. The standard methods of discretizations (for example, finite element method) require a solution 10^5 - 10^7 equations, that is impossible on modern computers. Our method of a partition of the problem on two recurrent sequences of the problems allows overcoming this difficulty.

3. At the classical approach the displacements are defined. For a determination of stresses interesting for the engineer, it is required to fulfill the procedure of numerical differentiation. It on an order worsens exactitude of a solution. We offer a new setting of a problem in stress-tensor, free from this shortage.

4. It is required the reminder of huge arrays in the problems of a viscoelasticity at discretization on time. It conduces to disastrous accumulation of round-off errors. The method, offered by us, allows solving the problem of a linear viscoelasticity on the whole interval of time, not resorting to discretization on time.

5. The iterative methods, used at all stages of solving, have significant restrictions on convergence and require the large number of iterations. The method of "interior iterations", used by us, allows essentially to expand area of convergence of used standard iterative processes and considerably to reduce machine time of a realization.

A Fast Two-Grid Banded Matrix Iterative Scheme for Electromagnetic Scattering

Mizanur Rahman

Brunel University

We consider a two-dimensional problem of scattering of a time harmonic electromagnetic plane wave by an inhomogeneous conducting or dielectric layer on a perfectly conducting plate.

Using a radiation condition proposed in [1], the problem is reformulated as a uniquely solvable second kind, Lippmann-Schwinger type integral equations on the unbounded inhomogeneous layer.

We solve the integral equation approximately using a simple piecewise constant collocation method, leading to a full linear system of order N . An advantage of the collocation method is that the coefficient matrix has the structure $I - TD$, where I is the identity matrix, D a diagonal matrix and T a block-Toeplitz matrix. This structure leads to a very efficient matrix-vector multiply if iterative schemes are employed.

We present a fast iterative solution scheme which uses a simple two-grid method and carries out the required matrix-vector multiplication efficiently in $O(N \log N)$ operations using the FFT. We present some numerical results comparing the numerical solution obtained by the two-grid iterative scheme with approximate analytical solutions given in [1].

- ***Making wave with multi-symplectic collocation methods***

Sebastian Reich

University of Surrey

Based on the formulation of Hamiltonian PDEs as multi-symplectic systems, we discuss numerical methods that preserve the corresponding conservation law of symplecticity. Such schemes can be considered as the natural generalization of symplectic integrators to PDEs. We demonstrate that the associated conservation laws for energy and momentum are well preserved under a multi-symplectic discretization. Applications include nonlinear wave equations, generalized KdV equations, and nonlinear Schrödinger equations.

The numerical solution of one-dimensional phase change problems using an adaptive moving mesh method

M. Robertson¹ & J. A. Mackenzie

¹University of Strathclyde

An adaptive moving mesh method is developed for the numerical solution of an enthalpy formulation of heat conduction problems with a phase change. The algorithm is based on a very simple mesh modification strategy that allows the smooth evolution of mesh nodes to track interfaces. At each time step the nonlinear enthalpy equation is solved using a novel semi-implicit moving mesh discretisation which is shown to possess a unique solution. Numerical examples are given for a two-phase freezing problem, a model of a spot-welding process, and a three phase problem with a varying number of interfaces. These test cases demonstrate the accuracy and effectiveness of the overall strategy.

A Fast Trend Transform - FTT

Carl H Rohwer

University of Stellenbosch

Local Monotonicity is a complementary concept to that of an impulse, and defines local trend in a precise way. Order n algorithms can be constructed to decompose a given sequence into components of linearly decreasing resolution detail. They are almost fully vectorizable yet, equivalent to existing computationally expensive procedures in a strict and illuminating sense. Conceptual comparison with FFT and FWT is interesting.

Starting algorithms for some DIRK methods

Teo Roldan¹ & Inmaculada Higuera

¹Universidad Publica de Navarra

When differential equations are solved with implicit Runge-Kutta methods, the computational effort is dominated by the cost of solving the non-linear systems. That is why it is important to have good starting values to begin the iterations. In this paper we construct starting algorithms for some DIRK methods in the literature. Numerical experiments have been done in order to compare the initializers studied in this paper with others used in the literature.

Uniform convergence on layer adapted meshes

Hans-Goerg Roos

TU Dresden

We describe a general class of layer adapted meshes for which easy to check sufficient conditions for uniform convergence can be formulated. The theory allows a precise analysis of upwind finite differencing or linear/bilinear finite elements for 2D convection-diffusion problems with exponential layers.

Moreover, we present the first uniform pointwise convergence result for a singularly perturbed quasilinear problem for a scheme of Enquist-Osher type.

Divergence-free Raviart-Thomas Finite Elements for 2nd-order elliptic problems in 3D

R. Scheichl

University of Bath

In this talk we consider second order elliptic boundary value problems over three-dimensional domains and their discretisation by means of lowest-order Raviart-Thomas mixed finite elements on general tetrahedral grids. This leads to indefinite saddle-point systems for discrete velocity and pressure fields. The application we have in mind is the velocity-pressure formulation of groundwater flow comprising Darcy's Law coupled with an incompressibility constraint subject to mixed boundary conditions.

We derive a method for the solution of this saddle-point system which uses a basis for the subspace of divergence-free Raviart-Thomas elements to decouple the problem into a symmetric positive definite system for the velocity and a separate system for the pressure. This approach has been investigated in 2D before, but the literature in 3D is restricted to a paper by Hecht (1981) on the related Stokes problem, and a paper by Cai et al. (1998) for uniform rectangular grids. It is particularly useful for groundwater flow applications where the velocity is of prime interest. An additional advantage is that the decoupled velocity system is about 3 times smaller than the original saddle-point system.

The proof of existence of such a basis involves techniques from graph theory and algebraic topology. We demonstrate the advantages of our approach by some computational results using the appropriate Krylov subspace methods to solve the different systems.

Computation of evolutionary stable strategies for population models with chaotic states

S.W. Schoombie¹ & M.H. Ellis

¹University of the Orange Free State

We consider a certain nonlinear, age-structured population model which, for certain parameter values, leads to periodic and chaotic population densities. We describe a simple algorithm which enables us to calculate a evolutionary stable strategy value for one of the parameters, which can be used even when the associated population density is chaotic. Some results are shown.

Row ordering for frontal solvers

Jennifer A. Scott

Rutherford Appleton Laboratory

The frontal method can be very efficient for solving large sparse highly asymmetric linear systems on modern computer architectures because, in the innermost loop of the computation, the method exploits

dense linear algebra kernels. These are straightforward to vectorize and parallelize. However, unless the rows of the matrix can be ordered so that the frontsize is never very large, frontal methods can be uncompetitive with other sparse solution methods. We introduce a new class of row ordering methods that exploit the row graph of the matrix. Using practical examples from large-scale chemical process engineering, the new methods are shown to perform significantly better than existing techniques and to greatly enhance frontal solver performance.

Nonconforming Galerkin Methods Based on Quadrilateral Elements for Second Order Elliptic Problems

Dongwoo Sheen¹, J. Douglas, Jr., J. E. Santos & X. Ye

¹Seoul National University

Low-order nonconforming Galerkin methods will be analyzed for second-order elliptic equations subjected to Robin, Dirichlet, or Neumann boundary conditions. Both simplicial and rectangular elements will be considered in two and three dimensions. The simplicial elements will be based on P_1 , as for conforming elements; however, it is necessary to introduce new elements in the rectangular case. Optimal order error estimates are demonstrated in all cases with respect to a broken norm in $H^1(\mathcal{O})$ and in the Neumann and Robin cases in $L^2(\mathcal{O})$. Also we will discuss domain decomposition iterative procedures based on nonconforming elements.

Control operators and iterative algorithms for nonlinear data assimilation problems

V Shutyaev

Russian Academy of Sciences

A class of quasilinear evolution data assimilation problems is considered. It is required to determine an initial value and/or the right-hand-side function so that the solution of the problem minimizes a functional related to observational data. The necessary optimality condition is obtained in the form of a set of equations which link the main and the adjoint states, and some additional equalities. With the analysis of the so-called control operators, the theorems on solvability of such systems are proved in a scale of Hilbert spaces. The regularity of solutions is studied. Using the spectral properties of the control operators, classes of iterative algorithms for solving the systems derived are developed, the convergence conditions of these algorithms are studied, and the convergence rate estimates are derived. Numerical examples are presented.

Fast solution techniques for convection diffusion problems

David J. Silvester¹, D. Kay & Syamsudhuha

¹UMIST

In this talk we discuss the design of efficient finite element solution algorithms for steady convection-diffusion problems. Two key components are discussed in detail; an adaptive refinement algorithm based on a cheap and efficient a posteriori error estimator, and a fast solution technique based on multigrid. Our numerical results suggest that the rate of convergence of the iterative solver is independent of the mesh and the Peclet number.

Approximate factorization in time-dependent PDEs

Ben Sommeijer¹ & P.J. van der Houwen

¹CWI

The spatial discretization of a system of time-dependent PDEs leads to a stiff initial value problem (IVP). We will discuss implicit methods for the numerical solution of such IVPs. The resulting implicit relations will be solved by an approximate factorization (AF) technique in order to reduce the linear algebra work involved. We will discuss the convergence of the AF process and the stability properties of the resulting integration method (based on underlying methods of BDF, Rosenbrock and DIRK type). Finally, an application to a shallow water transport problem will be reported.

Experiments on the edge of numerical stability

E. Sousa¹ & I.J. Sobey

¹Oxford University Computing Laboratory

Our understanding about the behaviour of numerical solutions for evolutionary convection diffusion equations is mainly based on analysis of infinite domains situations with stability based on von Neumann analysis. Almost all practical problems involve physical domains with boundaries. For a number of numerical schemes with Dirichlet boundary conditions, the numerical algorithm can be used without alteration near a boundary. The development of higher order methods such as Quickest or second order upwinding (including schemes with flux limiters) can introduce difficulty near an inflow boundary, since for points adjacent to the boundary there are insufficient upstream points for the high order scheme to be applied without alteration. All of these methods use a finite iteration matrix and these matrices can be non-normal, meaning that eigenvalue analysis alone may not be a good indicator of practical stability.

We consider some higher order finite difference schemes and their practical stability analysis. We use both conventional eigenvalue analysis of the iterative convection-diffusion matrix and additionally use the L_2 norm of the matrix, to obtain sufficient practical stability conditions. We carry out numerical experiments on the region where the matrix norm predicts growth but the eigenvalues predict decay.

As might be expected, it is not just accuracy but also stability, which dominates solution of time evolution problems.

Numerical solution of a nonlinear eigenvalue problem arising in resonance problems in electromagnetism

Alastair Spence

University of Bath

Rayleigh's method for the solution of doubly period problems in electromagnetism produces a nonlinear eigenvalue problem of the form $A(\lambda, \alpha)x = 0$, where A is an $n \times n$ Hermitian matrix, $\lambda \in \mathbb{R}$, $\alpha \in \mathbb{R}^2$, and $x \in \mathbb{C}^n$. This talk is about the efficient numerical solution of such eigenvalue problems.

A natural approach is to think about using Newton's Method on $F(\lambda, \alpha) := \det(A(\lambda, \alpha)) = 0$, but evaluation of the derivatives of F are expensive using this formulation. We use an approach derived directly from the work of Griewank and Reddien (SIAM J. Numer. Anal. (1984), p176) to derive an efficient procedure for the location, accurate determination and path-following of solutions to $F(\lambda, \alpha) = 0$. Numerical results for an application will be given.

Simultaneous Simulation with Adaptive Triangulation Methods

Martin Staempfle

University of Glasgow

Numerical simulation of dynamical systems plays an important role in a vast range of applications covering many different aspects. The majority of dynamical systems can be modelled with ordinary differential equations and appropriate initial conditions. In addition, most systems depend on one or several system parameters.

In the first part of this contribution, new methods for simultaneous integration of multi-dimensional sets of IVPs are presented. Such sets of IVPs can be obtained by varying system parameters. Parameter variation methods are commonly used as a tool for system design and parameter optimisation. The parameter domain is triangulated with adaptive methods that include refinements as well as derefinements. To achieve the same precision, the computational cost of adaptive methods is much lower than that of regular triangulations. This is a crucial advantage since every point in the parameter domain corresponds to the possibly expensive solution of an IVP. A sophisticated data structure with active and passive grid points is used to avoid any integration overhead.

In the second part, the method is applied to a model describing the dynamics of a passenger vehicle. The model includes longitudinal and lateral motion, pitch and roll, and tyre forces. The vehicle dynamics is computed for a sample test drive with fixed initial conditions and prescribed wheel steering as an input signal. Simultaneous simulations are performed for several vehicle parameters that vary within certain intervals. The results can be used to study the behaviour of the side slip angle which is a measure for vehicle stability and thus passenger safety.

A moving mesh method for hyperbolic conservation laws

John M. Stockie¹, J. A. Mackenzie & R. D. Russell

¹Simon Fraser University

We present an adaptive method for solving hyperbolic problems characterised by steep fronts or shocks. Our approach combines the high resolution "wave propagation" algorithms of CLAWPACK (R. J. LeVeque, J. Comp. Phys. **131**, pp. 327-353, 1997) with a moving mesh that is chosen to equidistribute some measure of solution error. The primary difficulty in constructing an accurate and efficient algorithm is the choice of an appropriate iterative scheme for coupling the equations for the solution and the mesh, that preserves the conservation properties of the original equations. We illustrate the advantages of the method with several one-dimensional examples, including Burgers equation and the Euler equations of gasdynamics.

Non-smooth data error estimates for linearly implicit Runge-Kutta methods and applications to long-term behaviour

M. Thalhammer¹ & A. Ostermann

¹University of Innsbruck

Linearly implicit time discretizations of semilinear parabolic equations with non-smooth initial data are considered. We prove that the order of convergence on finite time intervals is essentially one and derive an error estimate for the derivative of the solution with respect to the initial value. Such error bounds are needed to study the question whether the continuous dynamics of a parabolic problem is correctly represented in its discretization. As an illustration, we show that exponentially stable

solutions are uniformly approximated by linearly implicit Runge-Kutta methods over arbitrarily long time intervals. From this, stability bounds for splitting methods are obtained.

Newton's Method in Floating Point Arithmetic and Iterative Refinement of Generalized Eigenvalue Problems

Françoise Tisseur

University of Manchester

We examine the behaviour of Newton's method in floating point arithmetic, allowing for extended precision in computation of the function and possibly unstable solution of the linear systems. The application that motivates this work is iterative refinement for the generalized and quadratic eigenvalue problems. We show that iterative refinement can be used to improve the forward and backward errors of computed eigenpairs.

The PDE Coffee Table Book

Lloyd N. Trefethen¹ & Kristine Embree

¹Oxford University Computing Laboratory

The PDE Coffee Table Book is a group project at Oxford, which we hope to complete in 1999, whose aim is to produce a beautiful A4-size book with about 70 two-page spreads giving high-level information about the most important and interesting partial differential equations. For example, there are pages on the heat equation, the wave equation, Black-Scholes, Navier-Stokes, Sine-Gordon, Kuramoto-Sivashinsky....

This is not a numerical book, and yet, because we want pictures on every page, a great deal of numerical computation is going into its preparation. In this talk we will outline where the project stands and hope to get some advice from the audience.

Exponentially-fitted Runge-Kutta methods

G. Vanden Berghe¹, H. De Meyer, M. Van Daele & T. Van Hecke

¹Universiteit Gent

Exponentially-fitted Runge-Kutta methods are constructed, which exactly integrate differential initial-value problems, whose solutions are linear combinations of functions of the form $\exp(\omega x)$ and $\exp(-\omega x)$, Error control and step control techniques are discussed. Numerical experiments show the efficiency of certain methods.

Volterra discrete equations : summability of the fundamental matrix

Antonia Vecchio

CNR, Istituto per Applicazioni della Matematica

We consider the Volterra discrete equation (VDE)

$$x_n = \sum_{l=n_0}^n a_{n,l} x_l + g_n, \quad n \geq n_0, \quad x_n, g_n \in \mathbb{R}^d, \quad a_{n,l} \in \mathbb{R}^{d \times d}$$

and the representation of its solution by means of the fundamental matrix $u_{m,n}$

$$x_n = g_n - \sum_{l=n_0}^n (u_{l+1,n} - u_{l,n}) g_l, \quad n \geq n_0,$$

It can be easily seen that, the summability of first difference of the fundamental matrix assures that $\|x_n\|$ is bounded provided that the forcing function g_n is bounded. Therefore it becomes very important to answer the question: *what conditions on the coefficients $a_{n,l}$ imply the summability of first difference of the fundamental matrix?* The answer to this crucial question is already known for convolution equations. Here we try to give an answer in the case of nonconvolution VDEs. We give some conditions which assure the summability of first difference of the fundamental matrix and are based on sign and monotonicity properties of the sequence of coefficients $\{a_{n,l}\}_{n \geq n_0}$ of the considered VDE. These conditions apply exclusively to scalar equations. Since VDEs arise from the application of numerical methods to Volterra integral (VIE) and integro-differential equations, we use the mentioned results for proving the boundedness of the global error of some linear methods for nonconvolution VIEs.

Stable numerical methods for non-linear neutral delay equations

R. Vermiglio¹ & L. Torelli

¹University of Udine

We consider nonlinear neutral delay differential equations in Hale's form and we derive numerical methods which preserve the stability behaviour of the analytic solution. The basic idea is to reformulate the original problem eliminating the dependence on the derivative of the solution in the past values. Our hypothesis on the original equation allow us to study both contractivity and asymptotic stability properties by using the theory of stability with respect to a forcing term. It is an alternative approach, which reveals itself to be quite interesting, since can be easily reproduced for the numerical solution too. We introduce a numerical procedure based on continuous Runge-Kutta methods, we discuss the uniform order of approximation and, finally, we present methods preserving the stability properties of the underlying equation.

Asymptotic Successive-Corrections, Compact Operator Methods for Two-Point Boundary Problems

Francisco R. Villatoro

Universidad de Malaga, Spain

Asymptotic Successive-Corrections Techniques are numerical methods of global error correction based on an asymptotic expansion of the truncation error terms of a numerical method. These methods are based on the modified equations of the finite difference method, which are infinite-order differential equations asymptotically equivalent to the numerical method. These techniques are applied to a compact operator, fourth-order accurate, finite difference scheme for two-point boundary value problems. Numerical high-order approximations, completely consistent with the asymptotic expansion of the global error, are used for both Dirichlet and Robin boundary conditions. The resulting family of

high-order numerical methods are very accurate as tested in several examples using the methods with fourth, sixth, eighth and tenth order of accuracy.

A symbolic algorithm for the reduction and numerical solution of Higher Index DAEs

J. Visconti

LMC-IMAG

We propose an efficient symbolic algorithm for computing the index and constraints of nonlinear higher index DAEs. It is based on some linear algebra, and therefore designed for DAEs in the (quasilinear) form $A(t,y)y' = b(t,y)$, with $y = [y_1, y_2, \dots, y_n]$, and A a singular square matrix, b a vector, of dimension n . Under convenient assumptions, the algorithm is proved to provide the uniform differentiation index and a set of algebraic equations describing the solution manifold. Then, the computed set of constraints can be used for the numerical solution of the initial DAE, as an overdetermined index one problem, following the approach of [1,2]. Such a symbolic pre-processing allows reducing significantly the number of equations to be handled by the numerical solver. The algorithm has been implemented in Maple V, and experimented for classical problems of the literature. The gain in time for the numerical solution will also be illustrated.

[1] S.L. Campbell, E. Moore - "Progress on a General Numerical method for Nonlinear Higher Index DAEs" - [J] Circuits Syst. Signal Process. 13, No.2-3, 123-138 (1994).

[2] P. Kunkel, Volker. Mehrmann - Regular Solutions of Nonlinear DAEs and their numerical determination - Numerische Mathematik, Vol. 79, 1998, pp. 581-600.

Preconditioning for indefinite linear systems

Andy Wathen¹, Malcolm Murphy & Gene Golub

¹Oxford University

Iterative methods are often the only feasible methods for solving linear systems with large dimension, and are particularly applicable for sparse or structured systems. For many systems preconditioning is necessary to obtain acceptably rapid convergence.

In this talk we will describe some simple theory which provides guidance on how one might construct preconditioners for indefinite matrices with a particular but common structure. The novelty of our approach lies in the fact that our preconditioners are in no sense approximations of the coefficient matrix nor its inverse, but nevertheless the 'ideal' preconditioned matrices have very few distinct eigenvalues and so convergence (or indeed termination) of an appropriate iteration occurs in a correspondingly few steps.

We will indicate how Babuska-Brezzi stability for saddle-point problems in partial differential equations leads to preconditioners of this type.

Use of potential vorticity as a variable in data assimilation

M. A. Wlasak¹, N. K. Nichols & I. Roulstone

¹University of Reading

The problem of data assimilation is to estimate the states of a system from observational data together with a mathematical or numerical model of the system. It is assumed that the states are subject to random errors with a known (unbiased) Gaussian distribution. One form of data assimilation, 3D VAR, involves the minimisation of a cost functional at a given time and aims to deliver the maximum likelihood estimate of the system states at that time. This cost functional involves the sum of two terms: a background error term and an observational error term. The background error term takes the form

$$J_b = (x - x_b)^T B^{-1} (x - x_b), \quad (\text{the equation})$$

with x representing the model variables, x_b the background, or prior value of the states, and B^{-1} the background error covariance matrix.

The background term dominates the behaviour. The aim is to transform this background term by a change of variable so that B^{-1} is block diagonal. The transformed states include a variable known as potential vorticity; a quantity which contains significant dynamical information. We show some of the behavior of potential vorticity in a nonlinear shallow water model under different flow regimes. We also describe two possible control transformations that use this dynamical quantity.

An algorithm for continuous minimax problems with constraints

Stanislav Zakovic¹, Costas Pantelides & Berc Rustem

¹Imperial College, London

An algorithm for the continuous minimax problem with constraints is presented. The initial problem is transformed into an equivalent equality constrained problem, and then interior point approach is used. To satisfy the equality constraint a logarithmic barrier function is used and special care is given to step size parameter to keep the variables within permitted boundaries. We conclude with showing and discussing some numerical results.

Edge Element Methods on Non-matching Grids for Time-dependent Maxwell Equations with Discontinuous Coefficients

Jun Zou¹, Z. Chen & Q. Du

¹The Chinese University of Hong Kong

This talk investigates an edge element method for solving time-dependent Maxwell equations with discontinuous coefficients in general three dimensional Lipschitz polyhedral domains. The subdomains of different media can be triangulated using non-matching finite element meshes, error estimates are presented. The convergence analysis relies on a new abstract framework for general nested saddle point problems, a novel compactness argument for establishment of discrete inf-sup conditions, a specific characterization of the trace space $H(\text{curl}; D)$, a new extension result for any $H(\text{curl}; D)$ functions in a Lipschitz domain.