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# Abstracts of Invited Talks

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## *Reduced-Order Modeling of Large Scale Dynamical Systems*

<sup>†</sup>**Zhaojun Bai** (<sup>†</sup>University of California, Davis)

The goal of reduced-order modeling of a large scale dynamical system is to replace such a system by an approximate small system, namely, with much smaller state-space dimension. An accurate and effective reduced-order model can be applied for steady state analysis, transient analysis and sensitivity analysis. As a result, it can significantly reduce design time and allow for aggressive design strategies. Such a computational prototyping tool would let designers try “what-if” experiments in minutes and hours, not days.

In recent years, a great deal of attention has been devoted to Krylov subspace based reduced-order modeling techniques. The surge of interest was triggered by the needs of numerical techniques for simulations of extremely large scale dynamical systems, such as VLSI circuit simulation. In this talk, we will begin with a review of successful Krylov subspace based techniques for linear dynamical systems, and present the recent progress in quadratic and quasi-linear dynamical systems. We will conclude with the needs and challenges of reduced-order modeling techniques for nonlinear dynamical systems. Numerical simulation results for dynamical systems arising in circuit simulation, structural dynamics, and microelectromechanical systems (MEMS) will be presented.

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## *Additive Multigrid Theory*

<sup>†</sup>**Susanne C. Brenner** (<sup>†</sup>University of South Carolina)

The convergence of the V-cycle multigrid algorithm is usually handled by a multiplicative theory where the iteration operator (matrix) is expressed as a product of operators measuring the effect of the multigrid algorithm on different grid levels.

In this talk an additive convergence theory for the V-cycle algorithm will be presented. This theory is effective for establishing the asymptotic behavior of the contraction number of the V-cycle algorithm as the number of smoothing steps is increased.

The following applications of the additive theory will be discussed:

- [(1)] a complete generalization of the classical V-cycle convergence theorem of Braess and Hackbusch to the case of less than full elliptic regularity,
- [(2)] convergence of V-cycle and F-cycle algorithms for nonconforming methods with a sufficiently large number of smoothing steps.

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## *Preconditioners for Saddle Point Problems Arising in Computational Fluid Dynamics*

<sup>†</sup>**Howard C. Elman** (<sup>†</sup>University of Maryland)

Discretization and linearization of the Navier-Stokes equations

$$\alpha \mathbf{u}_t - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \text{grad}) \mathbf{u} + \text{grad} p = \mathbf{f}$$

subject to incompressibility constraints

$$-\text{div} \mathbf{u} = 0$$

leads to linear algebraic systems in which the coefficient matrix has the form of a saddle point problem,

$$\begin{pmatrix} F & B^T \\ B & 0 \end{pmatrix} \begin{pmatrix} \mathbf{u} \\ p \end{pmatrix} = \begin{pmatrix} \mathbf{f} \\ g \end{pmatrix}.$$

In this talk, we describe the development of efficient iterative solution algorithms for this class of problems. In particular, we show how initial approaches used for the Stokes equations, such as the Uzawa algorithm, can be viewed as solvers for the Schur complement system, and we discuss the advantages of explicitly working with the coupled form of the block system above and using the Schur complement as a tool for developing preconditioners. We describe some new algorithms derived using this point of view, and we demonstrate their effectiveness for solving both the steady-state and evolutionary Navier-Stokes equations.

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## *Inertia-Controlling Factorizations for Optimization Algorithms*

<sup>†</sup>**Anders Forsgren** (<sup>†</sup>Royal Institute of Technology (KTH))

When solving smooth optimization problems by sequential quadratic programming methods or interior methods using exact second-derivative information, often a linear system of equations involving a large sparse symmetric indefinite matrix has to be solved at each iteration. This matrix is often referred to as the barrier KKT matrix or the KKT matrix, depending on if an interior approach is used or not. For simplicity, we refer to it as the KKT matrix below. The inertia of the KKT matrix reveals if the problem is locally convex at the current iterate. In the convex case, the KKT matrix always has the correct inertia, and in this situation an off-the shelf sparse factorization routine can be used, where the pivot selection is based on sparsity and numerical stability. In the nonconvex case, it is of interest to find out the inertia during the factorization process. This can be done by imposing an additional restriction on the pivot selection, based on controlling the inertia of the submatrix factorized so far. We describe the issues of an inertia-controlling factorization and describe our experiments with a particular implementation.

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*Spectral Methods for Discontinuous Solutions*

<sup>†</sup>**David Gottlieb** (<sup>†</sup>Brown University)

Spectral methods involve approximating the solutions of partial differential equations by Fourier series or orthogonal polynomials. The attractive feature of those methods is their high accuracy for smooth solutions. When the solutions are not smooth the formal accuracy deteriorates and Gibbs oscillations develop. However there is extensive computational evidence that spectral methods yield high order accuracy when applied to complicated interactions of shock waves with smooth flows. In this talk we will review the state of the art in applying spectral methods to nonsmooth problems. We will review first the approximation theory and discuss the resolution of the Gibbs phenomenon, its practical aspects and applications in several fields as medical imaging.

We will discuss discontinuous solutions of hyperbolic equations and especially new results concerning conservation properties of multidomain spectral methods.

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*The state-of-the-art in numerical methods for quadratic programming*

<sup>†</sup>**Nick Gould & Philippe Toint** (<sup>†</sup>Rutherford Appleton Laboratory)

In this talk, we will describe two new methods for large-scale nonconvex quadratic programming. The first is an interior-point trust-region method, which has proved capable of solving problems involving up to half a million unknowns and constraints. The second, an active-set method, is still under development, and is intended primarily for the case where a good estimate of the optimal active set can be predicted. Key linear algebraic aspects of both methods will be described, as will the results of tests on a large set of convex and nonconvex quadratic programming examples.

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*Hierarchical Matrices*

<sup>†</sup>**Wolfgang Hackbusch** (<sup>†</sup>Max-Planck-Institut Leipzig)

Hierarchical matrices ( $H$ -matrices) are a tool for approximating dense matrices associated with elliptic pseudo-differential operators. In particular, they are suited for the discretisation of integral operators as they appear, e.g., in the boundary element method. But  $H$ -matrices can also be used to represent the (fully populated) inverse of a finite-element stiffness matrix. The storage of an  $H$ -matrix of size  $n \times n$  amounts to  $O(n \log^\alpha n)$  where  $\alpha$  is a small number depending on the variant of the  $H$ -matrix (there are even variants with  $\alpha = 0$ ).

The important feature of  $H$ -matrices is the fact that not only the matrix-vector multiplication but also all

matrix operations (matrix-matrix addition, matrix-matrix multiplication and inversion) can be performed approximately. Again the operation cost is linear in  $n$  up to logarithmic factors.

The construction of an  $H$ -matrix is based on a block-cluster tree, which is close to the cluster tree using in the panel clustering method for the fast matrix-vector multiplication in boundary element methods. Given the set of degrees of freedom together with geometric information (e.g., support of the basis functions) a block partitioning can be computed. Each block is filled with a low-rank matrix. The rank is a parameter which can be used to obtain the desired accuracy (difference of the true matrix and the  $H$ -matrix). Since the details of the discretisation do not enter the algorithm, the construction is black-box like.

Requiring a second hierarchy concerning the low-rank matrices, one obtains the  $H^2$ -matrices which have a number of nice properties.

In the case of boundary element methods, one uses  $H$ -matrices to avoid the dense system matrix, which requires that the approximation is sufficiently well. In the case of finite-element applications, at least a preconditioner (e.g., of a Schur complement problem) can be constructed by means of a rough  $H$ -matrix approximation.

However, there are further applications where the standard reduction to the matrix-times-vector operation is not sufficient. Examples are the exponential of a matrix and the solution of Lyapunov's equation, which can be achieved by means of  $H$ -matrices.

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*Estimating global error for highly-oscillatory ordinary differential equations*

<sup>†</sup>**Arieh Iserles** (<sup>†</sup>University of Cambridge)

To err is human, but it takes a numerical analyst to enquire of the nature of the error.

In this talk we address the issue of global-error accumulation in the numerical solution of highly-oscillatory equations  $y'' + g(t)y = 0$ , where  $g > 0$  is large. We commence by rederiving a formula, originally due to Peter Henrici, which expresses global error in terms of local truncation and the underlying variational flow. This is specialised to linear oscillators through the use of WKB asymptotic formulae, affording us the opportunity (at the cost of some algebra) to predict how global error accumulates for classical Runge-Kutta and multistep methods. The answer is “disappointingly” and this can be confirmed by direct numerical experiments: thus, for the Airy equation  $y'' + ty = 0$ , letting  $h \rightarrow 0$ , the amplitude error of **every** fourth-order classical method accumulates in the interval  $[0, T]$  as  $cT^{13/4}$ , where  $c$  is a method-dependent constant.

Can we do better? Lie-group methods, like the Magnus scheme, are much better, but considerable more can be done. Combining the Magnus approach with

linearisation about rotating frame of reference, we derive a method which, for the Airy equation, delivers (in exact arithmetic) global error which (in constant-step implementation) decays at the same speed as the exact solution,  $cT^{-1/4}$ , regardless of the length of the interval. As  $T$  grows, we might have an arbitrarily large number of oscillations within a single step - and yet the global error goes on decaying!

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*Linear Sampling Methods for Inverse Boundary Value Problems in Potential Theory*

<sup>†</sup>**Rainer Kress** (<sup>†</sup>University of Goettingen)

Linear sampling methods have been recently suggested and developed by Colton and Kirsch for the approximate solution of inverse obstacle scattering problems, i.e., for inverse boundary value problems for the Helmholtz equation. We present analogues of these methods for the solution of inverse Dirichlet and Neumann boundary value problems for the Laplace equation. We will describe both the mathematical foundation and the numerical implementation illustrated through two-dimensional examples.

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*A Resonance-Free Reversible Scheme for Multiple-Timescale Dynamics*

<sup>†</sup>**B. Leimkuhler** (<sup>†</sup>University of Leicester)

Integration of nonlinear Hamiltonian systems underpins much of modern computational science, including celestial mechanics and molecular dynamics. In both of the latter applications, the systems are characterized by multiple timescales, meaning that a qualitatively important dynamic is manifest on a time interval much greater than the period of the fastest local oscillatory mode. In most cases, the long time-scale phenomena are what we are after, but it is difficult or impossible to model the slow and fast parts separately: the fast components over a long period of time contribute to the system evolution.

These fast modes complicate the use of standard numerical integrators. In most cases we find that the timestep is limited in proportion to the period of the fastest oscillatory component present. For example, for the enormously popular Störmer-Verlet method, the timestep restriction is about 4 timesteps per fast period. This stability restriction greatly limits the effectiveness of numerical integrators, and it is for this reason precisely that many interesting phenomena lie beyond the reach of simulation, even on the fastest computers currently available. Attempts to push the timestep up based on partitioning of the forces into fast and slow terms (e.g. multiple timestepping) encounter resonances at around the fast oscillatory period.

In this talk, I will describe a new family of “reversible averaging” (RA) methods applicable to certain classes

of multiscale dynamical models, which combines ideas of multiple timestepping and averaging and which allows stable integration with very long timesteps and without resonances. A key difference between the new “Reversible-Averaging” methods and others that have been previously proposed is that we propagate the “fast” and “slow” variables by entirely different numerical/analytical processes, taking advantage of an assumed variable decomposition. The described method is not symplectic, but it does preserve the time-reversal symmetry of a mechanical system. I will also consider the application of the new method to problems in gravitational dynamics and discuss its potential use in molecular simulation.

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*A second order method for an integro-differential equation with bad initial data*

<sup>†</sup>**C Palencia & E Cuesta** (<sup>†</sup>Universidad de Valladolid)

A linear integro-differential equation of convolutive type, with a fractional kernel, is discretized in time by a suitable fractional version of the BDF2. The analysis is done in a Banach space setting. It is shown that by means of an inconsistent starting procedure the method achieves second order of convergence for bad initial data. The analysis and the numerical experimentation show that the proposed starting procedure is the only possible one rendering the method of second order for bad initial data.

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*Multimodels in numerical approximation of partial differential equations*

<sup>†</sup>**Alfio Quarteroni** (<sup>†</sup>EPFL, Lausanne & Politecnico di Milano)

This lecture will address several instances of model reduction that are advocated to solve partial differential equations with numerical methods having low complexity. We will consider heterogeneous domain decomposition methods to solve advection-diffusion processes in the case of non-overlapping subdomains. We will also address the case of overlapping domains by a technique of virtual control. Then we will consider the coupling of models featuring different geometrical dimensions (e.g. 3D and 1D) for the solution of fluid-structure interaction problems arising from haemodynamics. Various examples of physical interest will be illustrated.

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*Particles in a Random Velocity Field*

<sup>†</sup>**Andrew Stuart & Hersir Sigurgeirsson (SCCM, Stanford)** (<sup>†</sup>University of Warwick)

The aim of this work is to find a mathematical model for the motion of particles in a turbulent velocity field, consistent with experimental observations about particle distributions; and then to use this model to study

the effect of particle collisions on particle distributions.

We describe a mathematical model in which the velocity field is modelled as a Gaussian random field, and the particles are assumed to move according to Stokes' law. The velocity field may then be viewed as the solution of a stochastic PDE. An algorithm for the time-integration of the coupled stochastic PDE-ODE is described, including the handling of collisions. Some analysis of the cost of collision detection is also presented.

The model is analyzed in the framework of random dynamical systems and shown to be well-posed; in addition a random attractor is shown to exist. By a combination of numerical simulation, exploiting the existence of a random attractor, and some analysis when a natural time-scale separation occurs, the particle distributions are studied, with and without collisions.

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*Stability of Gaussian elimination*

**†Lloyd N. Trefethen** (†Oxford University)

Since Wilkinson's landmark 1961 paper it has been known that Gaussian elimination fails for certain matrices, amplifying rounding errors exponentially and generating worthless results. Yet such matrices "never" arise in practice. Why not? We shall review the curious history of this problem and report on recent developments.

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*Solving Stochastic Optimization Problems on Computational Grids*

**†Stephen Wright, Jeff Linderoth & Alex Shapiro**  
(†Argonne National Laboratory / University of Chicago)

We discuss a software tool called ATR ("asynchronous trust-region") for solving two-stage linear stochastic programming problems with recourse on computational Grids. Grids are parallel computing platforms assembled from a distributed collection of workstations, PCs, and pieces of clusters and conventional parallel computers. We also discuss results of unprecedented quality for some difficult problems from the literature, which have been obtained with our solver by means of large sampled-average approximations.

Our solver makes use of software tools developed in the metaNEOS and Condor projects. Condor is a system that maintains a heterogeneous "pool" of computational resources, from which it harnesses unused cycles to perform large parallel computations. It provides the tools that allow this inexpensive, powerful, but messy collection of resources to be used as an effective computational platform. The MW runtime support library developed in the metaNEOS project enables implementation of master-worker algorithms on Condor platforms.

Our algorithmic approach is built on a bundle-trust-region approach. Subgradients are evaluated by solving the second-stage problems in parallel for a given set of first stage variables. However, because of the heterogeneous nature of computational grids, the possibility of "losing" second-stage evaluations on unreliable worker nodes, and the possibly slow communication times, it is important for the algorithm to be asynchronous. Accordingly, we have modified the trust-region approach so that it considers more than one candidate for a new iterate at a time, allowing the algorithm to make progress even when some of the subgradient evaluations are not completed promptly on the worker nodes.

In addition, we present results obtained for some challenging problems from the literature. Variance reduction techniques and large sample sizes are used to obtain high-quality approximate solutions to problems in which the number of scenarios is much too large to allow for exact solution.

## Abstracts of Contributed Talks

*Comparison of Autoregressive Models for Time Series Prognosis Basing on Wavelet and Fourier Analyses*

**†Mikhail Alexandrov, Mikhail Yudin & Denis M. Filatov** (†National Polytechnic Institute)

Two autoregressive models for time series prognosis are considered. Unlike the traditional approach (see [3]), these models use coefficients of given orthogonal decompositions instead of time series values themselves. The model construction consist in 1) orthogonal transformations on various time intervals, 2) calculation of regressive coefficients (i.e. model parameters) between certain decomposition coefficients, and 3) testing the significance of model parameters using a statistic criterion. This approach allows to find out how small-scale changes lead to large-scale ones. For this, an expert uses a decomposition coefficient of lower order as a function and decomposition coefficients of higher orders as arguments in the formula of autoregression. A selection of an order of the coefficients depends on scales that are interested to the expert. Fourier transformation and various wavelet systems are considered (see [2]), and some results of prognoses are discussed. The examples use the observation data obtained from the government of Mexico City (see [1]).

Keywords: Time series analysis, wavelet analysis, autoregressive model.

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- [2] Goswami, J., Chan, A. (1999): Fundamentals of Wavelets. Theory, Algorithms, and Applications. John Wiley and Sons.
- [3] Rozanov, Yu. (1988): Stochastic processes. Publ. House "Nauka", Moscow, Russia.

*Application of Alternating Decomposition Technique*

**†Mikhail Alexandrov & Mikhail Yudin (Moscow State Geological Prospecting Academy, Russia; judin@msgpa.msgpa.ru)** (†National Polytechnic Institute)

The decomposition approach for a solution of mass transportation equation in a complex unlimited medium is considered. This approach was proposed by Shwartz in XIX and it was essentially developed at the 80s for the problems of electromagnetic sounding [2,4]. Unlike mentioned geophysical applications we use the decomposition technique for non-stationary processes and besides we use additional decomposition for the solution of external problem. The convergence of alternative decomposition is investigated and corresponding

results are discussed for various parameters of equation and calculation scheme.

Two levels of decomposition are described in detail. For a global decomposition the total unlimited area must be presented as an internal limited area containing all inhomogeneous parts of the medium and an external unlimited area containing homogeneous or regular medium. The internal problem is solved numerically and the external problem - analytically. Several analytical solutions are used if external area contains unlimited piecewise constant sub-areas. A local decomposition consists in presentation of internal area as a set of small sub-areas reflecting various inhomogeneities. The boundary conditions for external and internal problems are determined as a result of the concordance of their solutions on every time-step by means of an iterative process. In the submitted work the external problem is solved by method of orthogonal transformation [3] and the local sub-problems by method of coordinate splitting [1].

The developed technique of decomposition essentially reduces the requirements to a computer resource. It allows to use ordinary personal computers for calculation of complex models of a medium that is demonstrated on some examples.

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[4] Yudin, M. (1982): Alternative method for a numerical solution of geoelectrical problems. USSR Acad. of Sc., Moscow, Izmiran, pp. 47-52.

*The Use of Splines in the Numerical Solutions of Differential Equations*

**†Eisa A Al-Said** (†King Saud University)

We consider using uniform spline functions to develop numerical methods for computing smooth approximations to the solution and its derivatives of second order boundary value problems. We study the convergence analysis of the methods and we show that the second order cubic spline methods produce better results than the quadratic spline methods of the same order. Also, we briefly discuss the use of spline methods for solving certain initial boundary value problems in partial differential equations. Numerical examples are presented to demonstrate our conclusions.

*A Spline Collocation Method for the Heat Equation on Smooth Boundaries*

**†Juha Anttila** (†University of Oulu)

This talk considers a boundary element collocation method for the two-dimensional heat conduction problem with vanishing initial condition and a given Neumann or Dirichlet type boundary condition. Certain choices of the representation formula for the heat potential yield boundary integral equations of the first kind, i.e., the single layer and the hypersingular heat operator equations. The application of the theory of parabolic pseudodifferential operators makes it possible to analyze the collocation method for equations under concern in the case of general smooth boundary curve. In the analysis, the collocation equations are reduced to an equivalent Galerkin type problem by applying the well known Arnold-Wendland Lemma. For the discretization, general or quasiuniform meshes are applied and tensor products of the smoothest spline functions of arbitrary high odd degree (space) and continuous piecewise linear splines (time) are used as trial functions. Stability and convergence properties of the method are proved in appropriate anisotropic Sobolev spaces.

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*Supraconvergence of piecewise linear semi-discretizations for time-dependent problems with non uniform triangulations*

†**Silvia Barbeiro & J. A. Ferreira** (†Universidade de Coimbra)

We study the convergence properties of the semi-discrete approximations for parabolic problems defined on two dimensional polygonal domains. These approximations are constructed using a nonstandard piecewise linear finite element method based on non uniform triangulations of the domain and considering a variational formulation with a sesquilinear form which can be not strongly coercive.

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*On the numerical solution of singularly perturbed PDEs using moving mesh methods*

†**George Beckett, John Mackenzie, Alison Ramage & David Sloan** (†University of Strathclyde)

Numerical experiments are described that illustrate some important features concerning the performance of moving mesh methods for solving singularly perturbed partial differential equations (PDEs). The particular method considered here is an adaptive finite difference method based on one of the moving mesh methods proposed by Huang, Ren, and Russell [SIAM J. Numer. Anal. 31 (1994) pp.709-730]. This talk shows how the accuracy of the computations on adaptive meshes depends on the choice of monitor matrix, and a monitor matrix is presented which yields an optimal rate of convergence. An algorithm for the solution of the moving mesh system is presented in which the mesh equations are uncoupled from the physical PDE. The accuracy of various formulations of the al-

gorithms are considered and a robust time-step control mechanism is presented.

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*Inverse iteration and iterative solvers*

†**J. Berns-Müller** (†University of Bath)

Inverse Iteration is a popular algorithm for the matrix eigenvalue problem with well understood convergence properties. If direct solvers are possible, e.g. in situations where LU decomposition can be used, and accurate approximations to the desired eigenvalues are known, inverse iteration is usually the method of choice, often enhanced by versions using subspaces. However, for large scale problems derived from discretised PDE's, direct solvers are not computationally feasible and iterative methods for the linear solves must be considered. Hence we obtain a strategy which uses inexact linear solves, an **inner iteration**, within each step of inverse iteration, the **outer iteration**. The inexact solve depends on some threshold parameters which effect the work per **inner iteration** and also the quality of information provided to the **outer iteration**.

In this talk we present some basic convergence results for the case of inexact linear solves. Further an analysis of strategies for parameter selection will be presented with the aim of reproducing the same asymptotic convergence rate of inverse iteration with exact linear solves. Based on this analysis estimators are obtained which can be used for actual computations. Numerical examples illustrating these results will be presented.

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*The linear rational collocation method with iteratively optimized poles for two-point boundary value problems*

†**Jean-Paul Berrut & Hans D. Mittelmann** (†Université de Fribourg)

In the present work we propose, and discuss with numerical examples, an algorithm that improves upon the polynomial pseudospectral method for solving two-point boundary value problems (BVPs).

The version of the pseudospectral method we have in mind is that consisting of replacing the solution by an interpolating polynomial in Lagrangian form between well-chosen points and collocating at those same points. Since such points are vertical projections on the interval of points (nodes) equidistant or nearly equidistant on the circle, they accumulate in the vicinity of the extremities of the interval. As a consequence, the method is well-suited for solving problems whose solutions have boundary layers. Correspondingly, however, the center nodes are about equidistant, and farther from each other than the same number of equidistant nodes on the whole interval. As a consequence, the pseudospectral method has a hard time approximating solutions with large gradients (shocks)

away from the extremities of their domain of definition.

We present here a method that improves on the pseudospectral (polynomial) method without any change in the interpolation/collocation points and preserves the infinite differentiability of the solution. The idea is to modify the trial functions by attaching a denominator to the polynomial so as to make it a rational interpolant. The denominator is then successively optimized in an iterative procedure, with each step consisting of the solution of two problems: an optimization of the denominator for given values of the approximation to the solution at the interpolation points, and a collocation in the linear space of the rational interpolants with the just obtained, fixed denominator, to obtain new approximate values of the solution.

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*Sparse Approximate Inverse Smoothing and Modified Restriction Operator for Multigrid Solution of Nine-Point Approximations for Convection-Diffusion Problems*

<sup>†</sup>**Muddun Bhuruth & Sameer Sunhaloo** (<sup>†</sup>University of Mauritius)

Using central-difference approximations for solving convection-dominated flows, the use of coarse grid levels in the multigrid method may violate the fine mesh restrictions imposed by the cell Reynolds number. Various strategies for improving the robustness and efficiency of the multigrid technique for convection-diffusion problems have been proposed. However, these techniques fall short of attaining the efficiency observed for diffusion problems.

Recent work has shown that a high-degree of robustness can be achieved by multigrid techniques based on nine-point discretizations of two-dimensional problems while also yielding discrete solutions having a higher accuracy. Two essential components for a successful multigrid calculation are: the smoothing and the coarse grid correction techniques used. Often used smoothers are the Jacobi and Gauss-Seidel methods. In this talk we compare the performance of these smoothers with a sparse approximate inverse smoother. We also investigate the performance of the sparse approximate inverse smoother in conjunction with a recently proposed method which enforces the fourth-order accuracy at all coarse grid levels. Numerical results show that the sparse approximate inverse and the modified restriction operator yields higher convergence rates.

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*Mass Conservation and Moving Meshes*

<sup>†</sup>**Kenneth Blake** (<sup>†</sup>University of Reading)

Presented is a moving mesh method in 1-D using equidistribution and conservation of mass. Taking advantage of properties of the partial differential equation, the method is derived such that the solution values are

entirely dependent on the current grid and a quantity related to the chosen monitor function. The grid is found by solving a system of simple ordinary differential equations and bypasses any calculation or reference to a mesh in computational space. Numerical results are shown in reference to the porous-media equation and a similar problem related to semi-conductor processing.

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*Preconditioning via a Schur Complement Method - an Application in State Estimation*

<sup>†</sup>**Luise Blank** (<sup>†</sup>RWTH Aachen)

In chemical engineering complex dynamic optimization problems have to be solved on-line. We present a multiscale approach based on wavelets. Each discrete problem has to be solved only with an accuracy comparable to the current approximation error. Hence, we use an iterative solver also for the systems of linear equations that arise. Using properly scaled wavelets the condition numbers can be kept bounded independently of the refinement level. However, the smallest singular values are still close to zero due to inherent features of the estimation problem. The original problem is often ill-posed, the measure of observability of the model is typically low and the ODE's involved are stiff.

We suggest also applying a Schur complement technique with a -to our knowledge- new perspective. Namely, we eliminate respectively increase the smallest eigenvalues by computing the Schur complement with respect to a subspace, which captures the corresponding eigenvectors. Using the underlying infinite dimensional but wavelet discretized system, we determine the very low dimensional subspace, i.e. a coarse, adaptive grid, which captures approximately the eigenfunctions corresponding to the smallest eigenvalues. Due to the multiscale representation one expects that after the truncation to finite dimensional subsystems this coarse wavelet space still captures good approximations of the relevant eigenvectors. Indeed, all numerical experiments confirm this. The method provides an effective preconditioner and the numbers of iterations are drastically reduced.

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*Finite Element Method for Solution of Elliptical Equations*

<sup>†</sup>**I.V. Boikov & A.I. Boikova** (<sup>†</sup>Penza State University)

The first part of this paper is devoted to investigation the optimal with respect to accuracy methods of solutions of elliptic equations.

To this end at first it is investigated smoothness of solutions of elliptic equations. It is to be proved that under sufficient general assumptions solutions of the elliptic equations belong to ...

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For solution of elliptic equations there are constructed calculating schemes by finite element method and is proved optimality with respect to accuracy one of these scheme.

The second part is devoted to approximate solution of some problems of geophysics.

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*Numerical aspects of diffraction coefficient computations*

**†Bradley Bonner, I G Graham & V P Smyshlyaev**  
(†University Of Bath)

The computation of diffraction coefficients for the scattering of high-frequency waves by conical scatterers can be reduced to the solution of a family of homogeneous boundary value problems for the Laplace-Beltrami-Helmholtz equation on a portion of the unit sphere bounded by a simple closed contour (in fact the intersection of the sphere with the conical scatterer). Distance on the contour is geodesic distance on the sphere. The diffraction coefficient may be determined by then integrating the resulting solutions with respect to the wave number ([1]).

In this talk we discuss the numerical computation of the diffraction coefficients using the boundary integral method, with the classical double layer potential approach. The evaluation of the kernel of the integral equation involves computing the (derivative of the) Legendre function with complex index and for this we employ a method which combines solving Legendre's differential equation (when this equation is not singular), together with suitable asymptotic expansions near singular points.

An analysis of the kernel shows its relation to the kernels of the double layer potential for the planar Helmholtz and Laplace equations. This allows us to prove stability and convergence for a class of Nyström (or discrete collocation) methods. A question of key practical interest in this field is the computation of diffraction coefficients when the scatterer has edges and corners. Here we adapt well-known methods for handling boundary integral equations on planar corner domains ([2]) to the current problem. We illustrate the talk with computations on non-smooth scatterers.

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*Collocation methods for Volterra functional equations with (nonlinear) variable delays and nonsmooth solutions*

**†Hermann Brunner** (†Memorial University of Newfoundland)

A crucial step towards a complete analysis of the optimal convergence properties of collocation solutions for Volterra integral and integro-differential equations with state-dependent delays consists in understanding the effects of nonlinear (but state-independent) delays and weak kernel singularities on the attainable "classical" order of convergence in piecewise polynomial collocation methods for these less complex problems. In this talk I shall show that many results obtained for constant delays do not remain valid for second-kind integral equations (and integro-differential equations) with nonlinear delays. For first-kind Volterra equations (which arise in the discretization of certain neutral functional integro-differential equations of Volterra type) many of these questions remain open; I shall outline the difficulties inherent in the analysis and point out possible ways for overcoming them.

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*Numerical Stability for Stochastic ODEs*

**†Alan Bryden & Desmond J Higham** (†University of Strathclyde)

In this talk I will consider the linear stability of numerical methods for stochastic differential equations (SDEs). I will be focusing on asymptotic stability of the stochastic theta method whilst looking at how the results compare with those for deterministic problems. A new result concerning boundedness of asymptotic stability regions will be presented. I shall assume no background knowledge in SDEs.

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*Adaptive methods for scale invariant ODEs*

**†Chris Budd, Ben Leimkuhler & Matthew Piggott** (†University of Bath)

Many ordinary differential equations of mathematical physics are invariant under changes of scale and can admit (possibly singular) self-similar solutions. We show how to construct adaptive multi-step discretizations of these systems which admit the same scaling invariances as the original. These discretizations have discrete self-similar solutions which uniformly approximate the true self-similar solutions for all time and have the same stability characteristics. As a result certain singular systems can be computed with uniform accuracy as the singularity is approached. We demonstrate this by applying these methods to a problem of gravitational collapse.

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*The A-stability of methods with Padé and generalized Padé stability functions*

**†J. C. Butcher** (†The University of Auckland)

Some stability results are surveyed including the theorem formerly known as the ‘Ehle conjecture’. The use of ‘order stars’ is a powerful technique that has been successful in resolving many difficult stability questions; settling the Ehle result was one of its early successes. A slight variant of this approach, using what we call ‘order arrows’, can also be used to study questions about the possible A-stability of a numerical method, and we illustrate this in the case of the Ehle result. A discussion of the so-called ‘Butcher-Chipman conjecture’ includes a proof of a partial result.

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*Numerical Solution of Stefan Problems in Annuli*

**†Jim Caldwell & C.C. Chan** (†City University of Hong Kong)

Change of phase occurs naturally in many physical and industrial processes. The classical phase change problem is that of melting or solidification via the conduction of heat, which is referred to as the Stefan problem in the literature. The main difficulty in solving the Stefan problem is the presence of a moving phase boundary. Across the phase boundary the heat flux is not continuous, and the heat equation is replaced by a flux condition which relates the velocity of the phase boundary and the jump of heat flux across the phase front.

There are two main approaches to the solution of Stefan problems. Firstly, front-tracking methods such as the Heat Balance Integral Method (HBIM) provide a means of tracking the phase front explicitly. Secondly, using a fixed-domain formulation, the computational domain is fixed via a change of variable. A common approach here is the enthalpy formulation, which uses an enthalpy function together with the temperature as dependent variables.

In this work a novel enthalpy formulation is applied to the Stefan problem in annuli and is compared to the HBIM. The methods are applied to inward and outward solidification in cylindrical geometry, and the results are combined to give numerical solutions in annuli. It is found that the enthalpy method gives comparable accuracy to the HBIM except for small Stefan number, and is more efficient and flexible.

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*An efficient way to avoid the order reduction of Runge-Kutta type methods for nonlinear problems*

**†M. P. Calvo, J. de Frutos & J. Novo** (†Universidad de Valladolid)

In [1] a strategy to avoid the order reduction of Runge-Kutta methods for linear initial boundary value problems has been proposed. In this talk we investigate the applicability of such a technique to deal with nonlinear problems. More precisely, we show how the order reduction phenomenon can be efficiently avoided for

Burgers’ equation when the time integration is performed using a linearly implicit Runge-Kutta method. [1] M.P. Calvo and C. Palencia, Avoiding the order reduction of Runge-Kutta methods for linear initial boundary value problems”, Math. Comput. to appear.

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*The numerical solution of the singular integro-differential equations in Lebesgue spaces*

**†Iurie Caraus** (†Moldova State University)

In this report the numerical schemes of the collocation method and quadrature method for approximate solution of the singular integro-differential equations were elaborated. The case are investigated, when the equations defined on the arbitrary smooth boundaries, which closed in complex spaces. The theoretical foundation of these methods was given in Lebesgue spaces.

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*An Example of Failure in a Predictor-Corrector Algorithm for Linear Programming*

**†Coralia Cartis** (†University of Cambridge)

The Primal-Dual Predictor-Corrector (PD-PC) algorithm is an interior point method for linear programming that generates a sequence of iterates by computing changes in both the primal and the dual variables. The iterates are feasible with respect to the equality constraints of the primal and the dual problem and strictly satisfy the inequality constraints. On every iteration, two directions are computed, in an attempt to follow the central path approximately to the solution. The predictor direction is the tangent direction to the central path and the corrector makes an adjustment for the error that occurs in the linear approximation to the central path. The resulting search direction is taken as the sum of the predictor and the full corrector direction. Line searches are performed along it in order to prevent the new iterate from getting too near the boundary of the inequality constraints. An example will be given, however, where for any initial choice of the centering parameter, the PD-PC algorithm fails to converge to the solution, due essentially to the choice of the search directions. We conclude that, instead of searching along straight lines, one should multiply the contribution from the corrector by the square of the steplength.

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*Parallel Implementation of a Block Algorithm for Matrix 1-Norm Estimation*

**†Sheung Hun Cheng & Nicholas J. Higham** (†Centre for Novel Computing)

We describe a parallel Fortran 77 implementation, in ScaLAPACK style, of a block matrix 1-norm estimator of Higham and Tisseur. This estimator differs from that underlying the existing ScaLAPACK code,

PxLACON, in that it iterates with a matrix with  $t$  columns, where  $t > 1$  is a parameter, rather than with a vector, and so the basic computational kernel is level 3 BLAS operations. Our experiments on an SGI Origin2000 show that with  $t = 2$  or 4 the new code offers better estimates than PDLACON with a similar execution time. Moreover, with  $t > 4$ , estimates exact over 90% of the time are achieved with execution time growing much slower than  $t$ .

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*Finite-difference approximation of weakly damped nonlinear Shrödinger equation*

<sup>†</sup>**Raimondas Ciegis & V. Pakalnyte** (<sup>†</sup>Vilnius Gediminas Technical University)

In this article we consider one-dimensional nonlinear Shrödinger equation. The equation includes an absorption term and the solution is periodically amplified in order to compensate the lose of the energy. The problem describes a signal propagation in optical fibers.

The finite difference method is used to discretize differential equations. It is proved that the well-known Crank-Nicolson scheme is unconditionally unstable for this problem. We propose a new finite difference scheme and prove its stability and convergence.

We also consider two split step finite difference schemes and prove that they converge with the first and second order accuracy, respectively. Numerical results are presented.

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*Implementation of Heirarchic hp-Finite Element Families for Maxwell's Equations on Hybrid Meshes*

<sup>†</sup>**Joe Coyle & Mark Ainsworth** (<sup>†</sup>University of Strathclyde)

In seeking finite element solutions to problems involving the time-harmonic (single frequency) Maxwell's equations such as in electromagnetic scattering, it is well-known that the use of vector-valued functions constructed so that each component is in the nodal-based  $H^1$ -conforming space is inappropriate. It is necessary to use the Galerkin discretisation of the space  $H(\text{curl}; \Omega)$  which inherently maintains tangential continuity across interfaces such as edges or faces shared by adjacent elements. Additionally, allowing for higher or non-uniform local order of approximation, it is essential to work with a hierarchic set of basis functions. Nédélec elements [1] represent an appropriate starting point from which to construct an hp-finite element space for use on hybrid meshes with these requirements. In practice, however, realisation of these properties is not straightforward (see [2] for the 2D case).

In this talk, we provide a methodology for implementation of a basis suitable for non-uniform and higher order approximation on hybrid meshes for solving the

time-harmonic Maxwell's equations. Additionally, we will present numerical results for model problems as well as give a detailed discussion of the conditioning of the hp-finite element discretisation on tensor product meshes in 2D and 3D.

[1] J. Nédélec. Mixed finite elements in  $\mathbf{R}^3$ . *Numer. Math.*, 93:pp 315 - 341, 1980.

[2] M. Ainsworth and J. Coyle. Hierarchic hp-Edge Element Families for Maxwell's Equations on Hybrid Quadrilateral/Triangular Meshes. *Computer Methods in Applied Mechanics and Engineering*, To appear.

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*New Preconditioners for Mixed Finite Element Formulations of Second-Order Elliptic Problems*

<sup>†</sup>**Catherine Powell & David Silvester** (<sup>†</sup>UMIST)

Mixed finite element discretisations of scalar, second-order, elliptic partial differential equations give rise to symmetric, indefinite linear systems. The associated coefficient matrices are typically large, sparse and ill-conditioned, features that motivate our interest in efficient iterative solution methodologies for this linear algebra problem. Since the eigenspectrum of the system matrix is mesh-dependent, standard iterative schemes are not robust with respect to mesh refinement. Effective preconditioners are thus required.

A variety of preconditioners have been suggested in the literature. Our focus is on the construction of preconditioners for the original, indefinite problem, to be applied in conjunction with a MINRES solver.

We consider the application of Raviart-Thomas finite elements to 2-D problems and review generic stability criteria for mixed methods. Careful analysis of the discrete formulation of the inf-sup condition then provides a theoretical link to optimal preconditioning strategies. Two broad classes of preconditioners are distinguished and some well-known examples reviewed. In addition, two alternative, theoretically optimal candidates are proposed and applied in simple numerical trials.

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*Efficient fast multipole method for low-frequency scattering*

<sup>†</sup>**Eric Darve** (<sup>†</sup>Center for Turbulence Research, Stanford University)

The Fast Multipole Method (FMM) is a numerical method which has found a wide acceptance in the scientific community. It is a fast summation method for potentials in  $1/r$  and has applications in many areas such as Laplace and Poisson equations, particle simulations, molecular dynamics, etc. Another application of the FMM to Maxwell and Helmholtz equations (kernel in  $\exp(ikr)/r$ ) was initiated by V.Rokhlin. However the derivation of the FMM for Maxwell/Helmholtz has two major drawbacks. First, the method fails when the size of the clusters becomes very small com-

pared to the wavelength. This problem is known as sub-wavelength breakdown. The second limitation is the fact that numerically the approximation error of the method cannot be reduced beyond about  $10^{-4}$  relative error even when the number of poles is increased. This is due to numerical instabilities which, when coupled to roundoff errors, lead to a divergence of the method as the number of poles is increased beyond a certain threshold. In particular these two limitations mean that the FMM cannot be used for computations where the distribution of points is highly inhomogeneous (discretization of small details on the surface of the object for example) or when high accuracy is required (because of cavity resonances for example). We have developed a new variant of the FMM with complexity  $n \log(n)$  which is based on plane wave expansions. This new formulation leads to a method which is stable at all frequencies (no sub-wavelength breakdown) and is arbitrarily accurate. This method is more efficient and mathematically simpler than previous methods. It is also more efficient than the traditional FMM for Maxwell/Helmholtz at high frequencies. Finally the method is applicable to potentials in  $1/r$  as well. Again it leads to a method which is more efficient (less floating-point operations) than the traditional FMM and the newer variants of the same algorithm such as the variant proposed by Cheng-Greengard-Rokhlin in Journal of Computational Physics vol. 155 (1999).

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*New Algorithms for Solving ODEs and PDEs*

<sup>†</sup>**M T Darvishi** (<sup>†</sup>Razi University)

A new preconditioning method and a multidomain scheme are investigated to reduce roundoff errors in computing derivatives using Chebyshev collocation methods (CCM). In this paper, these algorithms and their applications to solve linear ODEs and PDEs are presented.

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*Analysis of the Cholesky method for Solving the Symmetric Definite Generalized Eigenvalue Problem*

<sup>†</sup>**Philip I. Davies, Nicholas J. Higham & Françoise Tisseur** (<sup>†</sup>University of Manchester)

The Cholesky factorization approach to solving the symmetric definite generalized eigenvalue problem  $Ax = \lambda Bx$ , where  $A$  is symmetric and  $B$  is symmetric positive definite, is to compute a Cholesky factorization  $B = LL^T$  and solve the equivalent standard symmetric eigenvalue problem  $Cy = \lambda y$  where  $C = L^{-1}AL^{-T}$ . Provided that a stable eigensolver is used, standard error analysis says that the computed eigenvalues are exact for  $A + \delta A$  and  $B + \delta B$  with  $\max(\|\delta A\|_2/\|A\|_2, \|\delta B\|_2/\|B\|_2)$  bounded by a multiple of  $\kappa_2(B)u$  where  $u$  is the unit roundoff. We take the Jacobi method as the eigensolver and give a de-

tailed error analysis that yields backward error bounds potentially much smaller than  $\kappa_2(B)u$ . Our analysis and experiments also give insight into the popular Cholesky-QR method, in which the QR method is used as the eigensolver. We also argue that it is desirable to augment current implementations of this method with pivoting in the Cholesky factorization.

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*Stability and convergence of collocation methods for time domain boundary integral equations*

<sup>†</sup>**Penny J Davies & Dugald B Duncan** (<sup>†</sup>University of Strathclyde)

Time domain boundary integral formulations of transient electromagnetic scattering problems involve retarded potential integral equations (RPIEs). Various numerical methods have been used to try to solve RPIEs, but they often prove to be unstable. There are some convergence results for finite element formulations, but these schemes are complicated and expensive to implement for RPIEs. Collocation schemes are easier to implement, but little appears to be known about their stability and convergence. We present new results on stability and convergence of collocation schemes and discuss the effect of numerical quadrature.

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*Numerical treatment of a certain Volterra integral equation with multiple solutions*

<sup>†</sup>**Teresa Diogo & Pedro Lima** (<sup>†</sup>Instituto Superior Tecnico)

In this work we have considered the numerical solution of a Volterra integral equation with weakly singular kernel. Although for certain values of a parameter in the kernel this equation possesses an infinite set of solutions, we have been able to prove that the Euler's method converges to a particular solution. It is also shown that the error allows an asymptotic error expansion in fractional powers of the stepsize, so that general extrapolation algorithms, like the E-algorithm, can then be applied to improve the numerical results. This is illustrated by means of some examples.

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*On error bounds of finite difference approximations to partial differential equations - temporal behavior and rate of convergence.*

<sup>†</sup>**Adi Ditkowski, Saul Abarbanel & Bertil Gustafsson** (<sup>†</sup>Brown University)

This work considers a family of spatially semi-discrete approximations, including boundary treatments, to hyperbolic and parabolic equations. We derive the dependence of the error-bounds on time as well as on mesh size.

The question of the role of numerically imposed boundary conditions in the solution of parabolic and hyper-

bolic PDE's has been with us for many years. Many investigators have studied the effect of boundary conditions on the stability of the overall scheme, ( i.e. the 'inner algorithm' + boundary conditions ) In this context stability implies convergence of the scheme, at a fixed time  $t$ , as the mesh is refined. The question of the temporal behavior of the error was usually not considered.

Another important question is what happens to the overall accuracy of the numerical solution if the order of accuracy of the inner stencil is higher then the order of the boundary conditions. This problem has been tackled by Gustafsson.

In the present work we had considered a form of differentiation matrices, both hyperbolic and parabolic, which represent a fairly wide family of boundary condition formulation plus central inner schemes. We investigate the dependence of the error on time as well as on mesh size. Numerical experiments, demonstrate the validity of these bounds.

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*A new universal numerical approach to solving mathematical physics problems*

<sup>†</sup>**Isom N Djuraev** (<sup>†</sup>Samarkand State University)  
To appear

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*The use of a new sparse indefinite code in optimization packages*

<sup>†</sup>**Iain Duff** (<sup>†</sup>Rutherford Appleton Laboratory)

We first describe the design of MA57, a new HSL code for the solution of sparse indefinite systems of equations. We will sketch some aspects of the underlying algorithms and indicate the improvements and added functionality with respect to our earlier MA27 code.

We then examine the use of the code within large scale optimization packages. In particular, we study why the new code performs better than MA27 in all phases of solution by a factor of up to ten in execution time on the linear systems from a run of the KNITRO package but, on the same nonlinear problem, the optimization package using the new code performs noticeably more slowly. This leads us to discuss issues of numerical accuracy in the solution of ill conditioned linear equations and the control of stability.

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*Computational Issues in Welltest Analysis*

<sup>†</sup>**Dugald B Duncan & Yiqi Qiu** (<sup>†</sup>Heriot-Watt University)

Welltest analysis is used by the oil and gas extraction industry to determine important properties of reservoirs. In its simplest form a welltest consists of shutting-in the reservoir (closing the valve on the wellbore) and letting the pressure distribution settle. Then the valve is opened and the flow rate and pressure at the output from the reservoir are recorded to

give a time history of the pressure drop at the output as oil and/or gas flow out. A mathematical model of the welltest process is then compared to the data, and unknown parameters such as reservoir thickness, diffusivity and skin factor (a measure of drill damage around the wellbore) are adjusted until a good fit is obtained. We describe the computational issues and models used in this process. A related talk examines the use of overlapping grids in approximating the diffusion equation describing pressure in the reservoir.

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*A Fitted Mesh Method for a Class of Singularly Perturbed Parabolic Problems with a Boundary Turning Point*

<sup>†</sup>**Raymond K. Dunne, E. O'Riordan & G.I. Shishkin** (<sup>†</sup>Dublin City University)

A class of singularly perturbed time-dependent convection-diffusion problems with a boundary turning point is examined on a rectangular domain. The solution of problems from this class possess a parabolic boundary layer in a neighbourhood of one of the sides of the domain. A numerical method consisting of a standard upwind finite difference operator on a fitted mesh is constructed. It is shown that the numerical approximations generated by this method converge uniformly with respect to the singular perturbation parameter. Numerical results are presented that verify computationally the theoretical result.

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*Steady vortex flows obtained from a constrained variational problem*

<sup>†</sup>**Behrouz Emamizadeh** (<sup>†</sup>Iran University of Science and Technology)

We prove existence of steady two dimensional ideal vortex flows occupying the first quadrant, and containing a bounded vortex; this is done by solving a constrained variational problem. Kinetic energy is maximized subject to the vorticity being a rearrangement of a prescribed function, and subject to a linear constraint.

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*The solution of stiff differential-algebraic equations with a dichotomically stable integrator*

<sup>†</sup>**Roland England & René Lamour** (<sup>†</sup>The Open University)

A dichotomically stable discretization is important when solving stiff boundary-value problems (BVPs) in ordinary differential equations (ODEs). A dichotomically stable implicit Runge-Kutta method has been implemented in a variable step-size initial-value integrator (SYMIRK), using an explicit, 4-step, extrapolation formula both as a predictor, and to provide a local error indicator.

Similar considerations apply to stiff BVPs in differential-

algebraic equations (DAEs), which, in some cases, may be thought of as the limiting case of stiff ODEs. Considerable modifications are required to the integrator, and in particular, the discretization must be expressed in terms of approximations to the derivative of the solution, rather than to the solution itself.

For index-one DAEs, such modifications have been carried out to the ODE integrator (SYMIRK), and a DAE integrator (SYMDAE) has been produced. This has been inserted into the multiple-shooting code (MSHDAE) developed by R. Lamour for differential-algebraic BVPs, replacing the standard BDF integrator which is not dichotomically stable.

For some stiff test problems, the standard version of MSHDAE fails to integrate across the interval of interest, but the new version using SYMDAE encounters no difficulty and produces an accurate solution. Indeed the efficiency of the process improves with increasing stiffness. For some non-stiff problems, the solution is also entirely satisfactory.

An optimal-control problem from chemical engineering has been formulated in terms of DAEs, involving a singular arc where the system is of index three. By introducing a singular perturbation, this may be thought of as the limiting case of a stiff index-one BVP in DAEs. It is hoped to report the results of the application of MSHDAE to this optimal-control problem.

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*Evaluating infinite range oscillatory integrals using generalised quadrature methods*

<sup>†</sup>**Gwynne Evans** (<sup>†</sup>De Montfort University)

The use of generalized quadrature methods based on Lagrange's identity has allowed a wide class of finite range irregular integrands to be easily integrated given a weight function  $w(x)$  which belongs to  $C^2[a, b]$  and which is the solution of an ordinary differential equation, say  $Lw = 0$ . Theoretical considerations have resulted in theorems as to the validity of the process, in particular these theorems give conditions under which the process is stable.

Applying the same philosophy to infinite range problems, which arise in practise in such widely different fields as financial stock market prediction and chemical reaction problems, has resulted in less than satisfactory results. The conditions for stability appear to break for the infinite range problem. Several approaches are presented here to overcome the difficulties. The direct approach is demonstrated to illustrate the difficulties, and two alternatives are presented. One involves using transformations to a finite interval so bringing the original methods into play. The choice of transformation appears critical to the success to this method. The second involves a subdivision strategy in which the infinite range generalised rule is used primarily as a mop-up rule to integrate say  $[N, \infty]$ , with

the convention finite rule being employed for  $[a, N]$ .

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*A new method for minimizing the condition number of a matrix*

<sup>†</sup>**D R V Fadrani** (<sup>†</sup>University of Tehran)

In this paper is considered a new method for the problem of minimizing the spectral condition number of a matrix. This problem arises in the construction of optimal feedback control for descriptor systems as well as in the construction of optimal preconditioners.

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*Balanced Flows in Models for Numerical Weather Prediction*

<sup>†</sup>**Steven J. Fletcher, Nancy K. Nichols & Ian Roulstone** (<sup>†</sup>University of Reading)

The task of predicting the weather involves the solutions to many nonlinear differential equations. Simplifications are made to these equations through balance approximations and scaling analysis. In these approximations, certain terms in the original equations are omitted and errors are introduced into the model dynamics. Data assimilation (DA) is one method for correcting the model errors. This technique uses observations of the weather system and compares these with the forecast from the numerical model to obtain a correction to the predicted states of the system.

Most of the features we wish to represent and predict in Numerical Weather Prediction (NWP) can be characterized as balanced. Properly constraining the assimilated solution to be near balance is essential to make the best use of incomplete observations. We describe here the application of balance constraints, derived from Hamiltonian mechanics, to a variational form of DA (VAR) which is currently used at The Met. Office. The constrained model solutions satisfy a linearised Monge-Ampère equation which is elliptic. The elliptic properties of the equation are shown to be sensitive to the approximations used in the case where the equations are applied on the sphere.

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*Approximation of Stable and Unstable Manifolds by Fixed and Variable Step-size RK Methods*

<sup>†</sup>**Paul Fenton & A.R. Humphries** (<sup>†</sup>University of Sussex)

Variable step-size numerical algorithms for solving ODEs based upon embedded RK pairs and a form of local error control are considered.

The existence and uniqueness of the local unstable manifold about a fixed point  $u^*$  in  $\mathbb{R}^d$  for ODEs is a well-known result.

When the step-size is fixed, it has also been proved that a consistent RK method has a uniquely defined local unstable manifold of  $u^*$ ; and that it is close to the underlying local manifold of the ODE. We extend this result to a (un)stable manifold theorem for fixed

time-stepping RK methods.

However, if the step-size is varied during the integration, the concept of a local unstable manifold of  $u^*$  breaks down. It is therefore necessary to construct a so-called local unstable set within  $\mathbb{R}^{d+1}$  with one higher dimension to include the step-size variable. The structure of this invariant set is investigated and it is shown that the ODE's local unstable manifold and the local unstable set are close for all embedded RK pairs in Hausdorff metric.

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*Alternating Decomposition Method and its applications to solving partial differential equations*

**†Denis M. Filatov, Mikhail A. Alexandrov & Mikhail N. Yudin** (†National Polytechnic Institute (IPN), Centre for Computing Research (CIC))

The classical problem of mass transportation (see [1]) with free boundary conditions is considered. Applying decomposition technique, we represent the total solution area as internal and external domains with non-empty intersection. The former contains various inhomogeneities and the internal problem is solved numerically; the latter is free of any inhomogeneities and sources, and the external problem is solved by analytical methods. We call this idea 'global decomposition' (see [3]). Iterative alternating process at every time step performs boundary value correction. Unlike well-known geophysical applications (see [2, 3]), we apply the decomposition technique to non-stationary processes, and besides, we have to perform additional correction for the external problems. Convergence of the iterative alternating process is studied and some appropriate results are discussed.

Keywords: Global decomposition, free boundaries, partial differential equations.

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*Vorticity-Streamfunction Dynamics and Numerical Resolution of Incompressible Viscous Flow*

**†Dalia Fishelov, M. Ben-Artzi & S. Trachtenberg** (†Tel Aviv University & Beit Berl College)

We consider the Navier-Stokes equations in vorticity-streamfunction formulation. The main difficulty associated with this formulation is that there is no boundary condition for the vorticity. We show that the

boundary conditions should be imposed on the streamfunction only, and the vorticity may be obtained via a projection of a function in  $L_2$  onto the space of functions, which are in the image of the Laplacian operator, with appropriate boundary conditions. The projection is carried out by a biharmonic equation, which relates the streamfunction to the Laplacian of the vorticity. Numerical results, including the lid-driven cavity, are shown.

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*On the Barzilai Borwein Method*

**†Roger Fletcher** (†University of Dundee)

The Barzilai Borwein method is a steepest descent method for unconstrained optimization that differs from the usual method in the way that the step length is chosen. Recent research has shown that it is competitive with conjugate gradients and has some advantages in some situations. It is capable of solving problems of  $10^6$  variables arising from 3D pdes in reasonable time. A feature of the method is its non-monotonic progress, which requires the use of a non-monotonic line search technique for non-quadratic problems. The talk will review the current situations and point to some open questions.

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*Balanced Flows in Models for Numerical Weather Prediction*

**†Steven J. Fletcher, Nancy K. Nichols & Ian Roulstone** (†University of Reading)

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*Solving Elliptic PDEs using Radial Basis Functions*

<sup>†</sup>**Bengt Fornberg & Elisabeth Larsson** (<sup>†</sup>University of Colorado)

In a collocation method, one starts by determining the coefficients in an expansion so that discrete data (e.g. a combination of function value and derivative information) becomes satisfied. In a Fourier pseudospectral (Fourier PS) method, we need the domain to be periodic and the data to be equi-spaced. Although the Chebyshev PS method allows the presence of boundaries, it still permits only minimal geometric flexibility. In contrast with this, collocation using smooth radial basis functions (RBFs) allows nearly complete geometrical freedom, while still featuring spectral convergence. Such RBFs usually incorporate a 'shape parameter', and we are here particularly interested in the limiting case of the basis functions becoming increasingly flat. We have found a numerical approach that largely overcomes the severe ill-conditioning that is traditionally associated with this situation. With this algorithm as our main computational tool, we use RBF collocation for solving Poisson's equation with Dirichlet boundary conditions. Three main variations for implementing RBF collocation for this problem have previously been proposed in the literature. We find that the accuracy in most cases increases dramatically when the shape parameter is brought to values that were previously 'off limits' for stable computations.

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*Visualization as a basis for discrete optimization for heat exchanger network synthesis*

<sup>†</sup>**Eric S Fraga, R Patel & G A Rowe** (<sup>†</sup>University College London)

Visualization techniques are typically used to present the results of numerical experiments. However, it is possible to use visualization for problem solving directly. This paper presents a visualization procedure for heat exchanger network synthesis. The user can interact directly with the graphical interface to improve the designs. More importantly, the visual representation is used directly as a discrete representation of the objective function. This objective function can be optimized automatically using a simulated annealing procedure. The use of a graphical representation as the basis for optimization provides the user with an intuitive interface to the optimization procedure, including the discretization parameters which are required by the procedure.

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*An energy-conserving discretization of the global shallow water equations*

<sup>†</sup>**Jason Frank** (<sup>†</sup>CWI)

The shallow water equations on the sphere are an important 2D model for atmospheric fluid dynamics. For spectral discretization via spherical harmonic ba-

sis functions, vorticity and divergence are commonly chosen as prognostic variables, since these quantities vary smoothly over the poles, in contrast to the velocity components. We first derive an energy conserving discretization based on the Hamiltonian form in velocity variables, and then apply a skew-symmetric change of dependent variables to obtain the vorticity-divergence equations. The resulting semidiscrete equations can be computed with just one extra spherical harmonic transformation.

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*High-order adaptive methods for nonlinear dissipative equations*

<sup>†</sup>**Javier de Frutos & Julia Novo** (<sup>†</sup>Universidad de Valladolid)

In this talk we present a technique for estimating spatial discretization errors of p-finite element solutions for nonlinear evolutionary dissipative equations in several space dimensions. Our approach can be included in the class of a posteriori estimates that have been called residual estimates. The error estimates are obtained by solving a discrete elliptic problem in a space of local polynomials of degree M

gt N if polynomials of degree N have been used to compute the Galerkin solution. The error estimate can be added to the spectral element solution to obtain a more precise approximation that has been called the postprocessed approximation and has been used in a different context to get an improved solution without increasing the computational cost. The calculation of the a posteriori error estimation is far less expensive than the computation of the numerical solution and can be carried out at every time when it is needed. The technique can also be applied to a finite-element space discretization. In this case the estimation can be carried out either with a refined mesh or with local polynomials of greater degree. The results can be used as a basis for an adaptive numerical procedure that controls adaptive enrichment through h or p refinement.

We use the method of lines procedure for solving the equations. A step-size selection strategy for some time integrators is coupled with the a posteriori error estimation for the p (h-p) refinement in order to control both temporal and spatial errors in the fully discrete scheme.

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*The Hertz Contact Problem, Coupled Volterra Integral Equations and a linear Complementarity Problem*

<sup>†</sup>**Alain Gauthier, Phil A. Knight & Sean McKee** (<sup>†</sup>University of Strathclyde)

This paper is concerned with the indentation of an elastic half-space by an axisymmetric punch under a monotonically applied normal force and under the assumption of Coulomb friction with coefficient  $\mu$  in the

region of contact. Within an inner (unknown) circle the contact is adhesive, while in the surrounding annulus the surface moves inwards with increasing load. In this paper it is shown how this problem is equivalent to two coupled Abel's equations with an unknown free point, the inner circumference of the annulus. It is further shown that a product integration finite difference approximation of those integral equations leads to a mixed linear complementarity problem (mixed LCP). A method based on Newton's method for solving non-smooth nonlinear equations is demonstrated to converge under restrictive assumptions on the physical parameters defining the system; and numerical experimentation verifies that it has much wider applicability. Results are compared with a more indirect approach due to Spence.

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*Discontinuous hp-Finite Element Methods on Shape-Irregular (anisotropic) Meshes*

**†Emmanuel Georgoulis & Endre Suli** (†University of Oxford)

We consider the hp-version of the discontinuous Galerkin finite element method (DGFEM) for second-order elliptic reaction-diffusion equations with mixed Dirichlet and Neumann boundary conditions. For simplicity of the presentation, we only consider boundary-value problems defined on an axiparallel rectangular domain whose solutions are approximated on subdivisions consisting of axiparallel elements. Our main concern is the generalisation of the error analysis of the hp-DGFEM for the case when shape-irregular (anisotropic) meshes and anisotropic polynomial degrees for the element basis functions are used. We shall present a general framework for deriving error bounds for the approximation error and we shall consider two important special cases. In the first of these we derive an error bound that is simultaneously optimal in  $h$  and  $p$ , for shape-regular elements and isotropic polynomial degrees, provided that the solution belongs to a certain anisotropic Sobolev space. The second result deals with the case where we have a uniform polynomial degree in every space direction and a shape-irregular mesh. Again we derive an error bound that is optimal both in  $h$  and in  $p$ . For element-wise analytic solutions the method exhibits exponential rates of convergence under  $p$ -refinement, in both cases considered. Finally, numerical experiments using shape-irregular elements for model problems exhibiting boundary-layer behaviour are presented.

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*Unstructured Domain Decomposition Methods*

**†Ivan G Graham & Eero Vainikko** (†University of Bath)

Domain decomposition techniques can be used to construct powerful preconditioners for PDEs discretised

on unstructured meshes. The preconditioner can be constructed automatically from the (element) stiffness matrices of the given problem, given only some basic information about the location of the freedoms. The coarse mesh component of the preconditioner need not have freedoms in common with the fine mesh and need not be based on the same type of elements but should in some sense reflect the quality of the fine mesh.

In this lecture we describe a parallel implementation of this technology, together with a brief description of its analysis and its use in the design of preconditioners for the incompressible Navier-Stokes equations.

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*Solving a sequence of sparse compatible systems*

**†Pablo Guerrero-Garcia & Angel Santos-Palomo** (†University of Malaga)

In this paper we describe how to maintain an explicit sparse orthogonal factorization in order to solve the sequence of sparse compatible systems needed to implement a non-simplex LP method similar to Gill, Murray and Wright's non-simplex method of early 90s. In order to do that, we have adapted to rectangular matrices (with more rows than columns) Saunders' techniques of early 70s for square matrices, by using the static data structure of George and Heath on early 80s but allowing row downdating on it. In this way we can take advantage of the intermediate results obtained when trying to  $\min \|A^T x - b\|_2$  by processing  $A^T$  row by row, in relationship with the LP in standard form  $\max b^T y$  subject to  $Ay = c$ ,  $y > 0$  by processing  $A$  column by column in the order dictated by a non-simplex method. We first justify the chosen factorization (the sparse QR factorization of  $A_k^T$ , where  $A_k$  is a subset of the columns of a fixed matrix  $A$ ), and then we give all the necessary formulae both if the orthogonal factor is available and if it is not. We also comment on our implementation on top of the sparse toolbox of Matlab 5.

**Key words:** sparse orthogonalization, Givens rotations, non-simplex methods, linear programming.

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*A non-simplex method for LPs in standard form*

**†Pablo Guerrero-Garcia & Angel Santos-Palomo** (†University of Malaga)

In 1973 Gill and Murray proposed a non-simplex method for the primal linear problem in inequality form  $\min(c^T x : A^T x > b)$ . In this paper a non-simplex method for its dual linear program in standard form  $\max(b^T y : Ay = c, y > 0)$  is given. A proof of its convergence is also included, as well as several comments on its implementation and on suitable phase-ones.

**Key words:** linear programming, non-simplex method, active-set method, phase I.

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*On the convergence of a radial basis function method*

for global optimization

<sup>†</sup>**Hans-Martin Gutmann** (<sup>†</sup>University of Cambridge)

Radial basis function interpolation has been successfully applied in a method that aims to find the global minimum of a continuous function. Numerical results show that it performs well compared to other global optimization methods. In this talk we discuss the theoretical convergence properties of the method using different types of basis functions, for example thin plate splines or multiquadrics. It turns out that an important role is played by the so-called native space that is associated with a particular basis function. Especially, it is of interest whether sufficiently smooth functions with bounded support are in the native space. We show that the native space can be characterized using Fourier transforms. This allows to derive sufficient conditions on the smoothness of a function for many choices of basis functions, e.g. thin plate splines. Then convergence of the global optimization method can be proved. For other basis functions, however, for example multiquadrics, it can be shown that the native space does not contain any function with bounded support. Thus convergence is still an open problem in these cases.

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*Computing the largest few singular values and vectors of highly ill-conditioned fundamental solution matrices of linear ODEs*

<sup>†</sup>**Raphael Hauser** (<sup>†</sup>University of Cambridge)

In numerical weather prediction one is often interested in the singular vectors corresponding to the largest few singular values of the fundamental solution matrix of the semi-discretized tangent-linear model of the equations of evolution around an operational orbit. These vectors yield information about the zones where new cyclones are forming and can be used in assessing the reliability of the operational weather forecast. The standard method for computing these vectors is Lanczos' procedure. We present a new algorithm with block-Lanczos type convergence, based on geometric integration of matrix-flow equations to compute a smooth singular value decomposition. Our new method overcomes ill-conditioning problems that are endemic in the standard method.

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*A numerical method for some stiff parabolic equations*

<sup>†</sup>**Gerald Hedstrom** (<sup>†</sup>LLNL, retired)

In 1983 Ray Chin and Robert Krasny proposed a robust method for stiff, stationary, 2-point reaction-diffusion problems, based on local linearization and adaptive gridding. In the early 1990s the author, along with Ray Chin and Fred Howes, extended the method to include convection. In the present paper a further extension is made to include time dependence.

*Stochastic ODEs and the One-Sided Lipschitz Condition*

<sup>†</sup>**Desmond J Higham, Xuerong Mao & Andrew M Stuart** (<sup>†</sup>University of Strathclyde)

Among the many highlights of the Dundee Conference series was Dahlquist's unveiling of a nonlinear stability theory for numerical ODEs based on the one-sided Lipschitz condition. To quote from Hairer and Wanner, **Solving Ordinary Differential Equations II**, 2nd Ed, Springer 1996, page 180:

*His search for a sufficiently general class of nonlinear systems was finally successful 12 years later. In his talk at the Dundee conference of July 1975 he proposed to consider differential equations satisfying a one-sided Lipschitz condition, and he presented some first results for multistep methods. J. C. Butcher (1975) then extended (on the flight back from the conference) the ideas to implicit Runge-Kutta methods and the concept of B-stability was born.* In this talk we will show how a one-sided Lipschitz condition can be used to establish finite-time, strong convergence of implicit numerical methods for nonlinear stochastic ODEs. Here the key difficulty is to obtain moment bounds for the numerical solution. No previous knowledge of stochastic ODEs will be assumed.

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*Computing the Nearest Correlation Matrix-A Problem from Finance*

<sup>†</sup>**Nicholas J. Higham** (<sup>†</sup>University of Manchester)

Given a symmetric matrix what is the nearest correlation matrix, that is, the nearest symmetric positive semidefinite matrix with unit diagonal? This problem arises in the finance industry, where the correlations are between stocks. For distance measured in a weighted Frobenius norm we characterize the solution using convex analysis. We show how the modified alternating projections method can be used to compute the solution. In the finance application the original matrix has many zero or negative eigenvalues; we show that the nearest correlation matrix has correspondingly many zero eigenvalues and that this fact can be exploited in the computation.

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*1D Model of a Fluid-Particle Mixture*

<sup>†</sup>**Adrian T Hill & W L Wan** (<sup>†</sup>Dept Mathematical Sciences, University of Bath)

Hill, Robinson, Sigurgeirsson, Stuart and Wan consider the equations of motion of several particles suspended in a fluid. Some of the difficulties of these equations are considered in the following one-dimensional model, which omits pressure and convection:

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Interestingly, exact estimates of the solution's regularity in  $C^{0,1}$  are required to prove uniqueness of solutions. Optimal error estimates for a Galerkin ap-

proximation are established in the spaces between  $L_\infty$  and  $C^{0,1}$ . However, in the  $L_2$  norm it is found that the Galerkin method yields an error which is suboptimal in the approximation theory sense. Numerical evidence and heuristic explanations are given for this phenomenon.

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*A multi-symplectic integrator of nonautonomous Hamiltonian PDEs*

**†Jialin Hong** (†Chinese Academy of Sciences)

It has been shown that the centred box discretization for Hamiltonian PDEs which don't depend explicitly on time and space variables is multi-symplectic. In senses of physics and other science fields, the Hamiltonian PDEs depending explicitly on time or space variables, so called nonautonomous, are more important. We define the multi-symplecticity for the nonautonomous Hamiltonian PDEs, and show that the centred box discretization is also multi-symplectic. The result is applied to numerical simulations of (periodically) quasi-periodically solitary wave for the variable coefficients KdV equation.

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*Hierarchical hybrid grids: A grid framework for high performance computing*

**†Frank Huelsemann** (†University of Erlangen-Nuremberg)

This work presents a novel grid framework for numerical simulation that combines the flexibility of unstructured grids with the high performance of structured ones. Hierarchical hybrid grids employ several grid levels which serve different purposes. The coarse and in general unstructured levels represent the geometry and the topology. The computations are carried out on highly structured refinements of the coarse grid elements.

The talk introduces the main concepts and demonstrates the performance gain for simple iterative schemes for linear algebraic systems. The experimental results from several computer platforms, ranging from workstations to supercomputers, underline the performance potential of hierarchical hybrid grids. The success of the approach has implications for the design of computationally efficient adaptive methods.

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*Travelling Waves (TWs) in Lattice Differential Equations (LDEs)*

**†Tony Humphries, K.A. Abell, C.E. Elmer & E.S. Van Vleck** (†University of Sussex)

LDEs are differential-difference equations defined by a system of ODEs coordinatized by a lattice. There is extensive theory and computation of TW solutions of parabolic type PDEs, but little beyond existence is known about TW solutions of spatially discrete analogues. Finding TW solutions of LDEs requires the solution of functional differential equation BVPs with

both advanced and retarded terms. We will discuss some of the issues involved in accurate numerical computation of these solutions using collocation methods. We will also present numerically computed TW solutions for several problems including Nagumo-type problems on uniform and non-uniform lattices.

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*Numerical Solution of the Windscreen Sagging Problem*

**†Roland Hunt** (†Strathclyde University)

The slumping of a thin sheet of very viscous liquid glass is used in the manufacture of windcreens in the automotive industry. The paper considers the numerical solution of thin viscous sheets having two free surfaces under gravity in both two and three dimensions. The forward solution is fairly straightforward but stability difficulties require the use of the backward Euler method in the time direction. However the interesting problem from an industrial viewpoint is the inverse problem, in which the viscosity profile is to be determined for a given shape. This is solved using an embedding problem in which a search is made amongst the family of forward solutions. The numerical difficulties involved for the inverse case will be discussed.

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*On the properties of some coefficients of multistep, multiderivative methods*

**†V Ibrahimov** (†Baku State University)

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*Preconditioning and parallel implementation of implicit Runge-Kutta methods*

**†Laurent O. Jay** (†The University of Iowa)

A main difficulty when implementing implicit Runge-Kutta methods for the numerical solution of ODEs and DAEs is to solve efficiently the systems of nonlinear equations. A new preconditioner for the iterative solution of these equations by the inexact modified Newton method will be presented. It consists of three steps: two involve the solution of linear systems and one involves matrix-vector products with the approximate Jacobian matrix. The major interest of this new preconditioner is that not only matrix decompositions can be executed in parallel, but the solution of linear systems can be done in parallel as well. For the Dahlquist test problem the preconditioner is asymptotically correct for the internal stages. On serial computers the decomposition cost of the preconditioner can be made equivalent to that of the implicit Euler method.

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*A new methodology for anisotropic mesh refinement based upon error gradients*

<sup>†</sup>**Peter Jimack, Thomas Apel, Sergei Grosman & Arnd Meyer** (<sup>†</sup>University of Leeds)

We consider a new strategy for controlling the use of anisotropic mesh refinement based upon the gradients of an **a posteriori** approximation of the error in a computed finite element solution. The efficiency of this strategy is demonstrated using a simple anisotropic mesh adaption algorithm and the quality of a number of potential **a posteriori** error estimates is investigated.

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*A finite volume/element approximation of the mean field model of superconducting vortices*

<sup>†</sup>**David Kay, C. M. Elliott & J. R. Claisse** (<sup>†</sup>University of Sussex)

In this talk a numerical scheme for the mean field model of superconducting vortices under the influence of a transverse magnetic field, is presented. A transverse magnetic field is applied, that reduces the problem from three dimensions to two dimensions. We must now find the scalar potentials for the vortex density and the magnetic field.

The arising system of two equations consists firstly of, a Hamilton-Jacobi type equation for the motion of vortex density inside the superconductor, and secondly, an elliptic equation posed on  $\mathbb{R}^2$ . The first equation involves a vortex pinning function.

A finite element method is implemented for the second equation, where a Dirichlet to Neumann mapping is used to reduce the computational domain of the problem onto one that is finite. For the first equation, a consistent and monotone scheme using finite volumes, that are linked to the finite element mesh, is used.

Numerical results are presented for arbitrary meshes and time dependent applied magnetic fields.

For a look at both one and two dimensional numerical results go to

<http://www.maths.sussex.ac.uk/Staff/DAK/SUP/super.html>

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*Pulse Detection in Initial Value Ordinary Differential Equations*

<sup>†</sup>**Patrick Keast, Amy Hynick & Paul Muir** (<sup>†</sup>Dalhousie University)

In many physical models ordinary differential equations (ODEs) arise in which abrupt changes of limited duration, known as pulses, can occur in the phase functions. These pulses may occur at times which are not known beforehand, and may have unknown durations. If the duration is sufficiently short, standard differential equation solvers will miss the pulse completely, stepping over it, especially if, prior to the pulse, the solution is well behaved. In this talk we discuss software which employs standard initial value ODE software and a process of defect sampling to at-

tempt to detect any pulses which arise.

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*How accurate is the streamline-diffusion FEM inside parabolic layers?*

<sup>†</sup>**Natalia Kopteva** (<sup>†</sup>Moscow State University & National University of Ireland)

A two-dimensional singularly perturbed convection-diffusion problem is considered. Its solution may have parabolic layers along the characteristic boundaries of the domain. It is shown that the streamline-diffusion formulation may, in the maximum norm, imply only first-order accuracy in parabolic-layer regions.

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*An Additive Schwarz Method For A Stationary Convection-Diffusion Problem*

<sup>†</sup>**A. Kerayechian & N. Ghahreman** (<sup>†</sup>Ferdowsi University of Mashhad)

In this paper, we discuss the solution of linear systems of algebraic equations that arise from the streamline method for a stationary convection-diffusion problem. We consider an additive Schwarz method applied to a linear, second order, nonsymmetric, indefinite problem. An alternative linear system, which has the same solution as the original problem, is derived and the GMRES method is used to solve this system. We show that the rate of convergence does not depend on the mesh size, nor on the number of local problems if the coarse mesh is fine enough.

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*A posteriori error estimation on anisotropic finite element meshes*

<sup>†</sup>**Gerd Kunert** (<sup>†</sup>TU Chemnitz)

Highly stretched, **anisotropic** finite element meshes can be advantageous to resolve solutions with strong directional features (e.g. boundary layers). On such anisotropic meshes, however, most of the conventional **a posteriori** error estimators fail because of the large aspect ratio of the finite elements.

Thus we have developed error estimators which are suitable also for **anisotropic** elements. A rigorous analysis shows that tight upper and lower error bounds can be achieved.

We present several error estimators for different problems and norms. The main ingredients are given and key issues are addressed. Numerical examples complement and confirm the analysis.

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*Adaptive timestepping for stochastic differential equations*

<sup>†</sup>**Harbir Lamba** (<sup>†</sup>George Mason University)

We describe a variable timestepping procedure for the pathwise (strong) numerical integration of stochastic ordinary differential equations with a single Brownian forcing. The algorithm is based upon embedded

Runge-Kutta pairs of strong order 0.5 and 1 that utilize only the low-order Stratonovich stochastic integral  $\int_{t_n}^{t_{n+1}} \mathbf{f}(\mathbf{x}_n) d\mathbf{W}$ . A new heuristic is developed for trying to optimise the chosen timesteps subject to satisfying the local error criterion, based upon an asymptotic analysis of the leading terms in the local error estimate. In particular the choice of stepsize is not constrained to be either half or double the previous attempted stepsize. The analysis highlights the potential unsuitability of the standard, analytically solvable, test problems for demonstrating the effectiveness of such algorithms on more general problems. Numerical results are also presented.

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*Finite element approximation of a sixth order nonlinear degenerate parabolic equation*

<sup>†</sup>**Stephen Langdon & John W Barrett** (<sup>†</sup>Imperial College)

In this talk we present a fully practical finite element approximation of the sixth order nonlinear degenerate parabolic equation

$$u_t = \nabla \cdot (b(u) \nabla \Delta^2 u)$$

where generically  $b(u) = |u|^\gamma$  for any given  $\gamma \in (0, \infty)$ . We also discuss an iterative scheme for solving the resulting nonlinear discrete system, and finally we present some numerical experiments.

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*Automatic generation of advection schemes*

<sup>†</sup>**Raymond Lashley** (<sup>†</sup>University of Reading)

A method has been developed for constructing conservative, shape preserving finite volume schemes on unstructured grids. These design criteria are motivated by the problem of tracer advection in a meteorological context where spurious negative values and generation/destruction are undesirable. Polynomial reconstructions of the local field are used to approximate fluxes and a flux limiter is applied to ensure shape preservation. The method has been designed to allow schemes to be generated automatically given the grid data and flow field. Greater accuracy is achieved, at an increased computational cost, by using higher order polynomials for the reconstruction.

The method has been applied to both regular and irregular grids on the plane and the sphere. Comparisons between accuracy and computational cost have been made for different orders of polynomials and grid resolutions to find the most ‘economical’ schemes. These vary between second and fourth order polynomial based schemes depending on the grid and the flow field being used. This talk will present a brief overview of the generation method and a discussion of the suitability of the resultant schemes for the advection problem in meteorology.

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*The numerical solution of the large-scale eigenvalue problem*

<sup>†</sup>**Richard B. Lehoucq, David Kay, Karl Meerbergen, Jennifer Scott & Andy Wathen** (<sup>†</sup>Sandia National Labs)

My presentation is about the effective solution of the large-scale linear systems that arise during a linear stability analysis.

The numerical solution of the steady state incompressible Navier-Stokes equations is an active area of research in computational science. Typically, the steady state solution is computed via a semi-discretized approach and a time integration. While tried and true, this approach does not readily allow the determination of unstable steady-states. Hence, a qualitative understanding of the dependence of the stability of a steady-state upon physical/discretization parameters is not feasible.

An alternative approach is to perform a non-linear solve for the steady-state combined with a linear stability analysis followed by a linear stability analysis. This is a classical approach that is not often attempted on complex three dimensional flows due to the nearly prohibitive computational requirements.

My presentation will review the numerical solution of the large-scale eigenvalue problem arising from a linear stability analysis of the steady state incompressible Navier-Stokes equations. I’ll then describe some of the details of an approach that uses an efficient Arnoldi based algorithm. My goal is to demonstrate the close relationship between transient based methods for determining the linear stability of fluid flow and the numerical solution of the eigenvalue problem arising from a linear stability analysis. In particular, I’ll examine how to construct the preconditioners needed by an iterative method for the linear systems that arise during the eigensolve.

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*How the Grinch solved MPECs - Mathematical Programs with Equilibrium Constraints*

<sup>†</sup>**Sven Leyffer, Roger Fletcher & Danny Ralph & Stefan Scholtes** (<sup>†</sup>University of Dundee)

Equilibrium constraints in the form of complementarity conditions, and more generally variational inequalities, often appear as constraints in optimization problems, leading to MPECs (Mathematical Programs with Equilibrium Constraints). The talk starts by reviewing some new applications of this modeling tool.

Over recent years, it has been argued that equilibrium constraints cannot be solved satisfactorily with standard techniques for Nonlinear Programming (NLP). Both numerical and theoretical evidence has been advanced which support this view.

We re-examine this assertion and present some startling numerical evidence which suggests that certain NLP

solvers can solve MPECs robustly and efficiently. We conclude by presenting some recent theoretical evidence which supports this view.

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*Low Rank Solution of Lyapunov Equations*

**†Jing-Rebecca Li & Jacob White** (†Courant Institute)

The Cholesky Factor ADI algorithm generates a low rank approximation to the solution  $X$  to the Lyapunov equation  $AX + XA^T = -BB^T$ . The coefficient matrix  $A$  is assumed to be large, and the rank of the right hand side  $-BB^T$  is assumed to be much smaller than the size of  $A$ . The Cholesky Factor ADI algorithm requires only matrix-vector products and matrix-vector solves by shifts of  $A$ . Hence, it enables one to take advantage of sparsity or structure in  $A$ .

It will be shown by numerical examples that the rational Krylov subspace generated by the Cholesky Factor ADI algorithm, where the shifts are obtained as the solution of a rational minimax problem, often gives the best approximation to the dominant invariant subspace of  $X$ .

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*Uniform methods for semilinear problems with an attractive turning point*

**†Torsten Linß & Relja Vulanovic** (†TU Dresden)

An upwind finite difference scheme is considered for the numerical solution of a class of linear and semilinear convection-diffusion problems with a small perturbation parameter  $\epsilon$  and an attractive (multiple) turning point. We show that for the scheme the maximum nodal error is bounded by a special weighted  $l_1$ -type norm of the truncation error. This result is used to establish  $\epsilon$ -uniform pointwise convergence on Shishkin meshes.

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*Analysis of preconditioners for saddle-point problems*

**†Daniel Loghin & Andy Wathen** (†Oxford University Computing Laboratory)

In this work we present an analysis of block-preconditioning techniques for the solution of sparse linear systems of equations resulting from mixed finite element formulations. Such problems lead to block matrices which afford efficient preconditioners if based on a similar block structure. Our aim is to characterize the performance of iterative solvers coupled with such preconditioning techniques. It turns out that the well-known Babuska-Brezzi conditions for the stability of our finite element formulation are sufficient both for the derivation and the analysis of block preconditioners. We present mesh-independent convergence bounds for various such preconditioners. In particular, we characterize Schur complement preconditioning for block matrices. We illustrate our analysis with examples arising in the finite element solution of problems from

linear elasticity and fluid flow.

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*$\epsilon$ -Entropy for Large Volume Limits of Discretized Parabolic Equations*

**†Gabriel Lord & Jacques Rougemont** (†Heriot-Watt University)

We examine statistical quantities of the global attractors of semi-discrete and fully discrete approximations of non-linear parabolic equations. We take the limit of unbounded domains which, by a scaling, is equivalent to the small viscosity limit. As a specific example we consider a Ginzburg-Landau equation with a Galerkin approximation in space and a time discretization that is exact for the linear part (a 1st order Strang type time splitting). We define spatial density of  $\epsilon$ -entropy, show that this is bounded and present some numerical results.

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*Finding small solutions to delay differential equations using numerical methods*

**†Patricia M Lumb & Neville J. Ford** (†Chester College of HE)

We review recent work which considers whether a non-autonomous delay differential equation has small solutions. Small solutions can cause problems for the analysis of delay differential equations and so their detection is an important issue. This talk shows how numerical methods can be used to give a visual method for detecting the existence of small solutions for a class of non-autonomous delay differential equations.

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*Sets of Fourier Coefficients using Numerical Quadrature*

**†James N. Lyness** (†Argonne National Laboratory and University of New South Wales)

One approach to the calculation of Fourier trigonometric coefficients  $\hat{f}(r)$  of a given function  $f(x)$  is to apply the trapezoidal quadrature rule to the integral representation

$$\hat{f}(r) = \int_0^1 f(x) e^{-2\pi i r x} dx.$$

Some of the difficulties in this approach are discussed. A possible way of overcoming many of these is by means of a polynomial subtraction" function. Thus, one sets

$$f(x) = h_{p-1}(x) + g_p(x),$$

where  $h_{p-1}(x)$  is an algebraic polynomial of degree  $p-1$ , specified in such a way that the Fourier Series of  $g_p(x)$  converges more rapidly than that of  $f(x)$ . To obtain the Fourier coefficients of  $f(x)$ , one uses an analytic expression for those of  $h_{p-1}(x)$  and numerical quadrature to approximate those of  $g_p(x)$ .

*The Numerical solution of the Phase Field Equations Using Adaptive Moving Meshes*

**†John Mackenzie, G. Beckett & M.L. Robertson** (†Strathclyde University)

An adaptive moving method is developed for the numerical solution of the phase-field equations. Distinguished limits of these equations include the classical Stefan model, its modification to include surface tension and surface kinetics, and the Cahn-Allen model of motion by mean curvature. The moving mesh method is based on a variational formulation and the governing equations are approximated using a moving finite element method. We will show how the mesh should be clustered to accurately follow solution interfaces. Numerical results will be presented for a planar travelling wave example and anisotropic crystal growth.

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*Numerical Solution Of Fredholm Integral Equation of The Second kind By Using Finite Element Method*

**†K Maleknejad & H Mesgarani** (†Iran University of Science & Technology)

In this paper we consider an adaptive finite element method for a Fredholm integral equation of the second kind. The algorithm produces a sequence of successively refined meshes with a final mesh on which a given error tolerance is satisfied. A reliable and efficient adaptive algorithm based on finite element method is then designed for a specific computational goal with applications to potential problems.

**Keywords :** Fredholm integral equation. Potential problems, Adaptive finite element method

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*Numerical solution of the Navier-Stokes equations using a compact-type method for constricting channel problems*

**†Paulo F. A. Mancera & R. Hunt** (†IBB/UNESP)

We present the numerical solution for the steady 2D Navier-Stokes equations using a fourth order compact-type method. The geometry of the problem is a constricted symmetric channel, where the boundary can be varied, via a parameter, from a smooth constriction to one possessing a very sharp but smooth corner allowing us to analyse the behaviour of the errors when the solution is both smooth or near singular. The set of non-linear equations is solved by Newton method. Results have been obtained for Reynolds number up to 500. Estimates of the errors incurred show that the results are very accurate and better than those of a second order method using central differences. Further the observed order has been shown to be close to four, for some Reynolds numbers.

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*Error Analysis of the Continuous QR Algorithm for Computing Lyapunov Exponents*

**†Ed McDonald & Des Higham** (†University of Strathclyde)

Lyapunov exponents give valuable information about long term dynamics. The continuous QR algorithm is a widely used numerical technique for computing approximate Lyapunov exponents, although it is not yet supported by a general error analysis. Here, a rigorous convergence theory is developed for the continuous QR algorithm applied to a constant coefficient linear system with real distinct eigenvalues.

We contrast results with those for the discrete QR algorithm. A key aspect of the continuous QR algorithm is that the stability, rather than the local accuracy, of the underlying timestepping algorithm is relevant, and hence the overall convergence rate is independent of the stepsize. In this case it is vital to use a timestepping method that preserves orthogonality in the ODE system. We give numerical results to illustrate the analysis.

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*Computing realistic Reynolds-uniform error bounds in the boundary layer for the numerical solution, and its discrete derivatives, of Prandtl's problem at high Reynolds numbers.*

**†John J. H. Miller, P.A. Farrell, A.F. Hegarty, E. O'Riordan, G.I. Shishkin** (†University of Dublin)

We describe a general experimental error analysis technique for computing realistic values of the parameter-uniform orders of convergence and error constants in the maximum norm associated with a parameter-uniform numerical method for solving singularly perturbed problems. We then employ the technique to compute Reynolds-uniform error bounds in the maximum norm for the numerical solution, and its appropriately scaled discrete derivatives, generated by a fitted-mesh upwind finite difference method applied to Prandtl's problem arising from laminar flow past a thin flat plate. Here the singular perturbation parameter is the reciprocal of the Reynolds number. This illustrates the efficiency of the technique for finding realistic parameter-uniform error bounds in the maximum norm for numerical approximations to the exact solution, and its scaled derivatives, of problems for which no theoretical error analysis is available.

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*Coupling Transport and Chemistry in Hyperbolic Equations*

**†Sarah Mitchell** (†University of Bath)

We consider a class of problems in which strong advection is combined with stiff source terms. Of particular interest is the study of the transport of chemical pollutants in groundwater flow. The key property of such systems is that the advected speed (i.e. speed of the chemicals in the groundwater) is typically retarded by a large factor depending upon the stiffness terms. Our

aim is to develop a numerical method that captures this aspect of the solution and is stable without too much restriction on the time step. In cases where there are various species in the model we may have a variety of speeds and varying degrees of stiffness in the relaxation terms resulting from a wide range of chemical reactions. The method should be able to cope with these different time scales without losing accuracy. We have studied systems with up to three different chemical species, and have developed a method that combines the box scheme and the trapezoidal scheme to deal with the advective and relaxation terms respectively. After changing the weighting in the spatial direction to damp oscillations we have a second order accurate numerical scheme which is unconditionally stable. A modified equation analysis of this discretisation shows how the reduced advected speed arises, and how the initial data is damped, and holds for a general relaxation term which is not necessarily stiff. This matches the time-asymptotic expansion analysis of the system which is restricted to considering only stiff relaxation terms (carried out by T-P Liu in 1987). The aim in future is to use this analysis of these simple coupled-equation models to investigate larger systems which are more physically realistic in modelling chemical processes with groundwater transport.

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*Single Cell Discretization of  $O(k^2 + h^4)$  for Fourth Order Nonlinear Parabolic Initial Boundary Value Problem of First Kind*

<sup>†</sup>**R.K. Mohanty & D.J. Evans** (<sup>†</sup>The Nottingham Trent University)

In this paper, we propose two new three level implicit difference methods of  $O(k^2 + h^2)$  and  $O(k^2 + h^4)$  in a coupled manner for the numerical solution of the one space dimensional nonlinear parabolic equation

$$A(x, t)u_{xxxx} + u_{tt} = f(x, t, u, u_t, u_x, u_{xx}, u_{xxx})$$

for  $0 < x < 1, t > 0$  subject to the initial conditions  $u(x, 0)$ ,  $u_t(x, 0)$  and boundary conditions  $u(0, t)$ ,  $u_x(0, t)$ ,  $u(1, t)$ ,  $u_x(1, t)$  are prescribed. Where  $h > 0$  and  $k > 0$  are mesh sizes in the x- and t-directions, respectively. In both cases, we use only (3+3+3)-grid points with a single computational cell and do not require to discretize the boundary conditions. The numerical solution of  $u_x$  is obtained as a by-product of the methods. We have also shown under appropriate conditions that the method is stable when applied to the model equation. Difference formulas for fourth order parabolic equation in polar coordinates are also discussed. We have also derived explicit schemes both for  $u$  and  $u_x$  of order four accuracy at first time level. Numerical results both for Cartesian and Polar coordinate problems are given to illustrate the methods and their convergence.

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*Conservative Schemes for Traffic Models*

<sup>†</sup>**J. Morgan** (<sup>†</sup>University of Reading)

There are a number of ways of modelling traffic flow, from statistical models to more fluid dynamic based approaches. The latter models are nonlinear differential equations, with flux functions which may be non convex, and require numerical solution. The schemes applied to these models need to be capable of capturing shocks, and are often of conservative upwind type. In this talk we discuss some of the models and schemes, and present some numerical results.

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*Inverse iteration and iterative solvers*

<sup>†</sup>**J. Berns-Müller** (<sup>†</sup>University of Bath)

Inverse Iteration is a popular algorithm for the matrix eigenvalue problem with well understood convergence properties. If direct solvers are possible, e.g. in situations where LU decomposition can be used, and accurate approximations to the desired eigenvalues are known, inverse iteration is usually the method of choice, often enhanced by versions using subspaces. However, for large scale problems derived from discretised PDE's, direct solvers are not computationally feasible and iterative methods for the linear solves must be considered. Hence we obtain a strategy which uses inexact linear solves, an **inner iteration**, within each step of inverse iteration, the **outer iteration**. The inexact solve depends on some threshold parameters which effect the work per **inner iteration** and also the quality of information provided to the **outer iteration**.

In this talk we present some basic convergence results for the case of inexact linear solves. Further an analysis of strategies for parameter selection will be presented with the aim of reproducing the same asymptotic convergence rate of inverse iteration with exact linear solves. Based on this analysis estimators are obtained which can be used for actual computations. Numerical examples illustrating these results will be presented.

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*A geometric convergence theory for preconditioned inverse iteration: New sharp convergence estimates*

<sup>†</sup>**Klaus Neymeyr & Andrew Knyazev** (**University of Colorado/Denver**) (<sup>†</sup>Universitaet Tuebingen)

Preconditioned gradient type eigensolvers are used to determine a modest number of the smallest eigenvalues and eigenvectors of extremely large symmetric positive definite eigenvalue problems. A new, recently presented geometric convergence theory inter-

prets such a scheme as a perturbation of inverse iteration. It provides a sharp, but lengthy convergence estimate.

In this talk, we present a new and much shorter convergence estimate for preconditioned inverse iteration, which is still sharp in the decisive quantities. The results hold for the generalized eigenvalue problem and for an associated subspace iteration scheme. The new estimates stimulate the search for new proof techniques that could be used to analyze such practically important improved preconditioned eigensolvers as the Locally Optimal Block Preconditioned Conjugate Gradient method. Numerical results are given for the Laplacian, which demonstrate the effectiveness of these preconditioned eigensolvers for mesh eigenproblems.

The talk is partially based on the paper:

A.V. Knyazev, K. Neymeyr, A geometric convergence theory for preconditioned inverse iteration. III: A short and sharp convergence estimate for generalized eigenvalue problems, SFB 382, Tuebingen, Report 161, April 2001.

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*Optimal control of an oscillating water column using both turbomachinery and relief valves*

<sup>†</sup>**N K Nichols, R.S. Gil & P.A.P. Justino** (<sup>†</sup>The University of Reading)

The aim is to maximize the power output from an OWC wave energy converter equipped with both turbine flow controls and relief valves. The system is modelled using realistic turbine characteristics that include losses and limitations. The numerical models approximate the hydrodynamic response of the pilot plant currently being tested on the Island of Pico in the Azores. The studies are carried out for both regular waves and irregular waves typical of sea states at the site.

The results show that the relief valve is optimally operated to prevent losses in turbine efficiency that can occur in high energetic sea states due to excessive pressure in the chamber. The action of the relief valve then leads to a significant increase in the energy generated by the device. Surprisingly, the operation of the valve at low pressures, in the case of both high and low energetic sea states, also acts to increase the power output. The improvement in energy generation is then more significant in lower energy sea states.

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*A Priori Estimates for the Global Error of ODE Solvers*

<sup>†</sup>**Jitse Niesen** (<sup>†</sup>University of Cambridge)

The global error of a time-stepping ODE solver is the difference between the computed and the exact solution, after a number of steps. In this talk, we show how to obtain **a priori** estimates for the global error. Our approach is based on perturbation theory and modified equations. The estimates are correct up

to a term of order  $h^{2p}$ , where  $h$  denotes the step size and  $p$  is the order of the method.

To illustrate the theory, we apply it to the nonlinear highly oscillatory equation  $y'' + ty^3 = 0$ . Using the asymptotic solution as  $t \rightarrow \infty$ , we estimate the global error committed by various Runge-Kutta methods. Numerical results confirm the correctness of our estimates.

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*Wavelet and Numerical Integrations*

<sup>†</sup>**Touraj Nikazad** (<sup>†</sup>Iran University of Science and Technology)

This paper deals with typical problems that arise when using wavelets in numerical analysis applications. The first part involves the construction of quadrature formulae for the calculation of inner products of smooth functions and scaling functions; we find a closed form. The second part of the paper deals with Wavelet integration method and compares it with other existing methods.

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*A numerical analysis of the incompressible Navier Stokes equations*

<sup>†</sup>**F Z Nouri & O Boutabou** (<sup>†</sup>Université Badji Mokhtar)

We consider the Navier Stokes equations for incompressible in a domain  $\Omega_d \in \mathbb{R}^3$ . When the velocity is sufficiently small we may neglect the nonlinear terms. We propose a numerical method which yields a solution to three dimensional problems by a finite number of two dimensional problems.

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*Householder's and Givens' transformations applied to complex vectors*

<sup>†</sup>**Gerhard Opfer** (<sup>†</sup>University of Hamburg)

If one applies a Householder transformation **H** which is written for the real case to a complex vector **x** one might be surprised: The matrix **H** is still orthogonal (in the sense  $\mathbf{H}\mathbf{H}^* = \mathbf{I}$ ) and  $\mathbf{u} := \mathbf{H}\mathbf{x}$  is (most likely) a vector as desired:  $\mathbf{u} = u_1\mathbf{e}_1$ , where  $\mathbf{e}_1 = (1, 0, \dots, 0)^T$  is the first unit vector. Of course this surprise will take place only if the code which is used allows complex arithmetic, like MATLAB, cf. [1, p.120], [2, p.249/250].

It turns out that the (advisable but not necessary) step one takes in the real Householder case to avoid cancellation, namely to make the calculation depend on the sign of the first component of **x** is a necessary step to make the computation right also in the complex case.

If one does the same with a (2x2)-Givens transformation **G** applied to a complex vector **x** one will be disappointed. The matrix **G** is not orthogonal anymore, however, the second component of  $\mathbf{u} = \mathbf{G}\mathbf{x}$  will still be annihilated. In order that the Givens transformation **G** (see [3, 253] for Givens rotation and [4, p.291]

for Givens reflection) also works in the complex case some changes are necessary.

There will be a discussion of both cases.

[1] J. W. Demmel: Applied numerical linear algebra, siam, Philadelphia, 1997, 419 p.

[2] G. Opfer: Numerische Mathematik für Anfänger, 3. Aufl. Vieweg, Braunschweig, Wiesbaden, 2001, 357 p.

[3] H. R. Schwarz: Numerische Mathematik, 4. Aufl. Teubner, Stuttgart, 1997, 653 p.

[4] J. Stoer: Numerische Mathematik 1, 8. Aufl., Springer, Berlin, 2000, 375 p.

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*Singularly perturbed differential equations with non-smooth data*

**†E. O’Riordan, P.A. Farrell, A.F. Hegarty, J.J.H. Miller & G.I. Shishkin** (†Dublin City University)

The location and strength of the layers in a singularly perturbed differential equation is influenced by the level of smoothness of the coefficients and source terms in the differential equation. Singularly perturbed ordinary differential equations of convection-diffusion type with discontinuous data are examined. The location and strength of the interior layers depends on the sign of the coefficient of the first derivative term either side of the point of discontinuity. Numerical methods based on monotone finite difference operators and piecewise-uniform meshes can be designed for these problems, whose numerical solutions are  $\epsilon$ -uniformly convergent.

---

*A second order method for an integro-differential equation with bad initial data*

**†C Palencia & E Cuesta** (†Universidad de Valladolid)

A linear integro-differential equation of convolutive type, with a fractional kernel, is discretized in time by a suitable fractional version of the BDF2. The analysis is done in a Banach space setting. It is shown that by means of an inconsistent starting procedure the method achieves second order of convergence for bad initial data. The analysis and the numerical experimentation show that the proposed starting procedure is the only possible one rendering the method of second order for bad initial data.

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*Incomplete Orthogonal Factorization using Givens Rotations*

**†Andreas T. Papadopoulos** (†Oxford University Computing Laboratory)

We explain, examine and present computational results for some incomplete Givens QR factorisation methods recently introduced as preconditioning methods by Z.-Z. Bai, I.S. Duff and A.J. Wathen (BIT 41(1), March 2001). Given a (sparse) nonsingular system

of linear equations, these algorithms produce an incomplete QR-type factorization of the original matrix. The factors can be used as preconditioners for any standard iterative method applied either to the original system or to the associated system of normal equations, in order to speed up its convergence. In this talk we will deal with two of these algorithms: the Incomplete Givens Orthogonalization (IGO-method), where the sparsity patterns of the resulting factors are determined by the sparsity pattern of the original matrix (dropping by position) and the Threshold IGO-method (TIGO-method) which drops entries dynamically by their magnitudes. In the first part of the talk we will concentrate on programming aspects and difficulties related to the implementation of these algorithms. In the second part, we will identify classes of matrices for which these methods can produce useful preconditioners without too high requirements. A comparative analysis of the performance of these methods against standard general incomplete LU type factorizations will also be presented, having chosen Saad’s SPARSKIT toolbox (also written in Fortran) as the opposing standard.

---

*Filtering out Boundary Reflections in Two Dimensional Hyperbolic Equations Using Coupled Waves Method of Analysis*

**†M.Parsaei** (†Tehran University)

When using finite difference method, to approximate two dimensional hyperbolic equations numerically, central differences are usually used in the mid nodes, while, at the non-physical boundaries upwind differencing is employed. This results in a reflection at these boundaries. A two dimensional coupled waves method of analysis determines the properties of the solution waves along the adjacent lines of nodes. If we apply this method to the middle nodes and the nodes next to the boundaries the reflection ratio of each component waves can be determined. Using these ratios, and a filtering mechanism, the amount of reflected waves at the boundaries can be reduced. In this method depending on the complexity of the shape of the boundaries different methods of coupling should be used. To cope with very complex shapes each section of the boundary can be analyzed separately and it’s part in producing the reflected waves can be determined.

---

*Solving the Indefinite Least Squares Problem*

**†Harikrishna Patel & Nicholas J Higham** (†University of Manchester)

The indefinite least squares problem is to minimize  $(b - Ax)^T J (b - Ax)$  with respect to  $x$ , where  $J = \text{diag}(I_p, -I_{m-p})$  and  $A \in \mathbb{R}^{m \times n}$ ; as a special case, the standard least squares problem is obtained for  $p = m$ . We discuss some properties of the problem

and then describe numerical methods. A stable but slow method has been given by Chandrasekaran, Gu and Sayed (1998). We look at faster ways of solving the problem with the aid of the hyperbolic QR factorization. The use of hyperbolic rotations and hyperbolic Householder matrices is discussed, as well as stability of these methods.

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*Tuning the parameters to frequencies in Runge-Kutta(-Nyström) methods for oscillatory problems*

†**Beatrice Paternoster** (†University of Salerno)

We consider numerical methods for  $y'' = f(x, y)$  having oscillatory solutions, in which the informations a priori known on the frequencies can be embedded. If the location of the frequencies are known in advance, we can *tune* the parameters of the methods to them, as proposed by Gautschi in 1961. In this talk we explore and compare three different approaches. We extend trigonometric collocation to two step Runge-Kutta methods, assuming that the dominant frequencies  $\omega_j$  are a priori given. We also derive a Runge-Kutta-Nyström (RKN) method which results exact in phase for linear problems with periodic solutions. Finally, only assuming that the frequencies are located in a given nonnegative small interval  $[\omega_1, \omega_2]$ , we adapt the parameters of the RKN method through least squares minimization.

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*The Development of an Adaptive Moving Unstructured Staggered Mesh Method for Incompressible Flows*

†**Blair Perot & Xing Zhang** (†University of Massachusetts)

A three-dimensional unstructured staggered mesh method is present which allows for an arbitrarily moving mesh. The mesh motion is used to track moving or free surfaces and to allow mesh concentration in regions with large solution errors. Local mesh flipping is used to reconnect the mesh when it becomes highly distorted. Anisotropic mesh smoothing is used to concentrate the mesh in regions of large estimated solution error and to adjust the interior mesh smoothly to boundary motions.

The method is shown to conserve volume, mass, momentum, and kinetic energy. The staggering of the mesh means that no pressure coupling terms are required and that the incompressibility constraint is satisfied to machine precision. An exact fractional step scheme, which has no splitting errors, is used to update the pressure. The method has been efficiently parallelized using MPI and implemented on a 60-node Beowulf cluster.

Calculations are presented of an oscillating droplet, the flow around a square cylinder, two-dimensional and three-dimensional free-surface sloshing, and droplets colliding with a wall. Comparisons are made with

both experimental data and analytical solutions.

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*Geometrical adaptive methods for the semi-geostrophic equations of meteorology*

†**Matthew Piggott** (†University of Bath)

In this talk we consider the use of adaptive methods in the numerical solution of PDEs. We introduce a problem from meteorology - the semi-geostrophic equations. This is a problem which may be written in terms of an advection equation coupled with a Monge-Ampère equation describing a coordinate transformation. This is a challenging problem to consider numerically, for example the equations support the formation of discontinuities (atmospheric fronts).

We will demonstrate links between the Legendre coordinate transformations used to study the semi-geostrophic equations and numerical concepts of adaptivity based on moving meshes. In particular we show how geometrical ideas play a key role in the numerical analysis of the system.

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*Numerical solution of the Navier-Stokes equations using a compact-type method for constricting channel problems*

†**Paulo F. A. Mancera & R. Hunt** (†IBB/UNESP)

We present the numerical solution for the steady 2D Navier-Stokes equations using a fourth order compact-type method. The geometry of the problem is a constricted symmetric channel, where the boundary can be varied, via a parameter, from a smooth constriction to one possessing a very sharp but smooth corner allowing us to analyse the behaviour of the errors when the solution is both smooth or near singular. The set of non-linear equations is solved by Newton method. Results have been obtained for Reynolds number up to 500. Estimates of the errors incurred show that the results are very accurate and better than those of a second order method using central differences. Further the observed order has been shown to be close to four, for some Reynolds numbers.

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*New Preconditioners for Mixed Finite Element Formulations of Second-Order Elliptic Problems*

†**Catherine Powell & David Silvester** (†UMIST)

Mixed finite element discretisations of scalar, second-order, elliptic partial differential equations give rise to symmetric, indefinite linear systems. The associated coefficient matrices are typically large, sparse and ill-conditioned, features that motivate our interest in efficient iterative solution methodologies for this linear algebra problem. Since the eigenspectrum of the system matrix is mesh-dependent, standard iterative schemes are not robust with respect to mesh refinement. Effective preconditioners are thus required.

A variety of preconditioners have been suggested in

the literature. Our focus is on the construction of preconditioners for the original, indefinite problem, to be applied in conjunction with a MINRES solver.

We consider the application of Raviart-Thomas finite elements to 2-D problems and review generic stability criteria for mixed methods. Careful analysis of the discrete formulation of the inf-sup condition then provides a theoretical link to optimal preconditioning strategies. Two broad classes of preconditioners are distinguished and some well-known examples reviewed. In addition, two alternative, theoretically optimal candidates are proposed and applied in simple numerical trials.

---

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*An error bound for polynomial interpolation to functions of several variables*

**†M.J.D. Powell** (†University of Cambridge)

Quadratic polynomial interpolation is used in a recent algorithm developed by the author for unconstrained minimization calculations, and an estimate of the error of the quadratic model is required. Fortunately, a development of Kowalewski's exact remainder provides an error bound in terms of the Lagrange functions of the quadratic interpolant and the greatest third derivative derivative of the objective function,  $M$  say. Further, a suitable approximation to  $M$  can be derived automatically by the algorithm from

function values. These techniques will be described. We note that the error bound can be generalised to interpolation by polynomials of any degree. This result is not original, however, and is given in the study of "multipoint Taylor formulae" by Shayne Waldron (Numerische Mathematik, 1998).

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*A new method for the numerical solution of backward parabolic problems*

**†José María Marbán Prieto & C. Palencia de Lara** (†Universidad de Valladolid)

A new method for solving numerically backward parabolic problems is proposed. As usual for this kind of ill posed problems, it is assumed that an *a priori* bound on the solution is available. The algorithm consists of two basic steps. First, a standard forward integration is performed, in order to approximate the solution at suitable future time levels. Second, a holomorphic recovery procedure is carried out, providing the required approximations for the preceding times. The analysis is valid in a Banach space setting and rigorous estimates are derived. Among other advantages, the method can also be applied to nonlinear problems and it produces a continuous output. Some numerical illustrations are presented.

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*Overlapping Grids for Welltest Analysis*

**†Yiqi Qiu & Dugald B Duncan** (†Heriot-Watt University)

The welltest analysis process is used to determine important properties of oil and gas reservoirs. A related talk deals with the general issues of welltest analysis. The heart of most welltest simulation and analysis software is a linear, transient diffusion model for pressure in the reservoir. In this talk we examine the use of overlapping grids in approximating the diffusion equation. They make it easy to build up the computational domain for complicated reservoirs in a modular fashion, using sub-grids fitted in an optimal way to the wellbore and geological features such as faults. We give results for fully implicit schemes on the overlapping grids and examine accuracy, convergence, efficiency and the choice of interpolation to link the solutions on different grids together.

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*Oscillations in Discrete Solutions of the Convection-Diffusion Equation*

**†Alison Ramage & Howard Elman** (†University of Strathclyde)

It is well known that discrete solutions to the convection-diffusion equation contain nonphysical oscillations when boundary layers are present but not resolved by the discretisation. For the Galerkin finite element method with linear elements on a uniform 1D grid, a precise statement as to exactly when such oscillations occur

can be made, namely, that for a problem with mesh size  $h$ , constant advective velocity  $w$  and different values at the left and right boundaries, oscillations will occur if the mesh Péclet number is greater than one. In 2D, however, the situation is not so well understood. In this talk, we present an analysis of a 2D model problem on a square domain with grid-aligned flow which enables us to clarify precisely when oscillations occur, and what can be done to prevent them. We prove the somewhat surprising result that there are oscillations in the 2D problem even when  $P_e < 1$ . Also, we show that there are distinct effects arising from differences in the top and bottom boundary conditions (equivalent to those seen in 1D), and the non-zero boundaries parallel to the flow direction. Finally, we use the analysis to characterise the effects of upwinding strategies on solution quality and to choose a streamline upwinding parameter which gives accurate solutions for problems with non-grid-aligned and variable speed flows.

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*Study of the stability of absorbing boundary conditions for the continuous Schrödinger problem*

<sup>†</sup>**Nuria Reguera & Isaías Alonso Mallo** (<sup>†</sup>University of Burgos, Spain)

In a large number of differential equation problems the spatial domain is unbounded. In practice, when solving numerically such a problem, it is necessary to reduce it to a bounded domain using artificial boundary conditions. For Schrödinger-type equations, the transparent or reflection-free boundary conditions (TBC) are nonlocal. For this reason, we develop a general class of absorbing boundary conditions (ABC) that approximate the TBC by considering rational interpolating functions. We denote these ABC by  $ABC(j_1, j_2)$ , where  $j_1, j_2$  are the degrees of the polynomials in the numerator and denominator of the rational function, respectively. We will call order of absorption the value  $j_1 + j_2 + 1$ .

The discretization of these problems is carried out by the method of lines. For the spatial discretization we use finite differences, obtaining a system of ordinary differential equations. We prove that the semidiscrete problem for  $ABC(1,0)$  is weak ill-posed. Nevertheless, the ill-posedness is very weak and  $ABC(1,0)$  may be useful in practice. We also show numerically that the semidiscrete problems associated to ABC of high order are worse posed. However, the worse behavior of higher order ABC can be cancelled because of the greater absorption at the boundary.

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*Stability of some nonlinear Volterra integrodifferential equations and their discretised versions*

<sup>†</sup>**Jason A Roberts, J.T. Edwards & N.J. Ford** (<sup>†</sup>Chester College)

We present new results concerning the stability of equations of the form

$$y'(t) = - \int_0^t k(t-s)\phi(y(s))ds, \quad t > 0$$

where the kernel  $k$  is a decaying exponential term (representing a fading memory system),  $\phi : \mathbb{R} \rightarrow \mathbb{R}$  is an odd function, and of a suitable discrete analogue.

We prove, using the direct (or second) method of Lyapunov (and using conditions on  $\phi$  that we have not seen elsewhere), that the equation above has a stable zero solution.

We then consider discrete versions of the form

$$y_{n+1} - y_n = -h^2 \sum_{j=0}^{n+1} \omega_j^{(n)} A_{n+1-j} \phi(y_j), \quad j \in \mathbb{N}$$

and give a corresponding analysis.

Finally, we illustrate our results with some numerical experiments.

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*A Chebyshev-based two-stage iterative method as an alternative to the direct solution of linear systems*

<sup>†</sup>**Daniel Ruiz & Mario Arioli** (<sup>†</sup>ENSEEIH)

We consider the solution of ill-conditioned symmetric and positive definite large sparse linear systems of equations. These arise, for instance, when using some symmetrizable preconditioning technique for solving a general (possibly unsymmetric) ill-conditioned linear system, or in domain decomposition of some numerically difficult elliptic problem. We are also concerned with the consecutive solution of several linear systems with the same matrix and changing right hand sides. In such cases, the consecutive runs of some iterative methods like the conjugate gradient or the block conjugate gradient algorithms might appear to be computationally prohibitive, and it might be preferable to use direct methods which are very well suited for this type of situation.

The purpose of our study is to analyse a two-phase approach: analogously to direct methods, it includes a preliminary phase which we may call “partial spectral factorization phase”, followed by a “cheap” solution phase, both only based on numerical tools that are usually exploited in iterative methods. Therefore, we can keep the given ill-conditioned matrix in implicit form through matrix-vector products. This is of particular interest in the case of very large sparse systems and for an efficient implementation in distributed memory architectures.

Combining Chebyshev iterations with the block Lanczos algorithm, we propose a way to identify and extract the precise information related to the ill-conditioned part in the given linear system, and to use it for the computation of extra solutions related to the same matrix and with changing right-hand sides. The potential of this combination, which can be related to

the factorization and direct solution of linear systems, is illustrated experimentally in the general case of preconditioned unsymmetric sparse linear systems.

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*Numerical Range of Block Matrices*

<sup>†</sup>**Abbas Salemi** (<sup>†</sup>Kerman University)

The notion of quadratic numerical range was introduced by H. Langer and C. Tretter. In this paper under some conditions we find some relationship between the quadratic numerical range of some block matrices and its numerical ranges. Also new concepts such as joint quadratic numerical range and mth numerical range is introduced.

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*Evolutionary games*

<sup>†</sup>**Schalk Schoombie & Michelle Erasmus** (<sup>†</sup>University of the Free State)

In certain population models it is possible to assign a parameter to a survival strategy. Using evolutionary game theory, which is a simple application of dynamical systems, it is sometimes possible to calculate an optimal strategy, known as an Evolutionary Stable Strategy (ESS).

We discuss some theoretical considerations which enable a simple algorithm for the numerical calculation of ESS's

Such an algorithm is essential in cases where the population is in a complicated periodic or chaotic state.

---

*A Multilevel Algorithm for Wavefront Reduction*

<sup>†</sup>**Jennifer A. Scott & Yifan Hu** (<sup>†</sup>Rutherford Appleton Laboratory)

A multilevel algorithm for reordering sparse symmetric matrices to reduce the wavefront and profile is described. The algorithm is a combinatorial algorithm that uses a maximal independent vertex set for coarsening the adjacency graph of the matrix and an enhanced version of the Sloan algorithm on the coarsest graph. On a range of examples arising from practical applications, the multilevel algorithm is shown to produce orderings that are better than those produced by the Sloan algorithm and are of comparable quality to those obtained using the hybrid Sloan algorithm. Advantages over the the hybrid Sloan algorithm are that the multilevel approach requires no spectral information and less CPU time.

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*A Fast Parallel Solver for the Biharmonic Problem*

<sup>†</sup>**David Silvester & Milan Mihajlovic** (<sup>†</sup>UMIST)

We examine the convergence characteristics of preconditioned Krylov subspace solvers applied to the linear systems arising from low-order mixed finite element approximation of the biharmonic problem. We de-

scribe a “black-box” multigrid preconditioning operator that is easily implemented and which leads to preconditioned systems having an eigenvalue distribution consisting of a tightly clustered set together with a small number of outliers. We present numerical results showing that the performance of this simple methodology is competitive with other fast iteration methods that have been proposed in the context of biharmonic problems.

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*Accelerating the Numerical Solution of Multi-term Fractional Differential Equations*

<sup>†</sup>**Charles Simpson & N.J. Ford** (<sup>†</sup>Chester College)

Integro-differential equations involving fractional differential operators are becoming increasingly common in mathematical models. Accurate, reliable and rapid algorithms for their approximate numerical solution are required.

Diethelm and Luchko have recently developed the work of Lubich, on convolution quadratures and fractional linear multistep methods, to produce an algorithm to solve linear multi-term fractional differential equations.

In our recent paper (to appear in Numerical Algorithms) we showed how the calculation of the approximate numerical solution of a single term fractional differential equation could be accelerated by using a system of nested meshes and demonstrated this by combining the nested mesh system with an algorithm of Diethelm.

Here we examine the outcome of combining a system of nested meshes with fractional linear multistep methods to linear multi-term fractional differential equations and compare the effectiveness of this approach with combining a system of nested meshes to the algorithm of Diethelm.

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*High order interpolatory integration on the sphere*

<sup>†</sup>**Ian H. Sloan & R.S. Womersley** (<sup>†</sup>University of New South Wales )

For some applications (e.g. geodesy) it would be useful to have interpolatory cubature formulae on the sphere that have positive weights and are of high degree  $n$ . By analogy with quadrature on an interval, these are formulae obtained by integrating exactly the interpolating spherical polynomial of degree  $n$ . But almost all choices of interpolation points on the sphere lead to very poorly conditioned linear systems, and/or to some of the weights being negative. In this work we introduce a new approach to this problem. This has already led to interpolatory cubature rules on the sphere that have all weights positive, and  $n$  as large as 128. In the latter case the rule has  $129^2 = 16,641$  well chosen points, and the  $16,641 \times 16,641$  dense matrix used to determine the weights has a small condition num-

ber. The design of such rules is a major exercise in computational optimization.

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*A Schur method for computing matrix pth roots*

<sup>†</sup>**Matthew Smith** (<sup>†</sup>University of Manchester)

Given a matrix  $A \in \mathbb{C}^{n \times n}$ , a matrix  $X$  is a  $p$ th root of  $A$  if  $X^p = A$ . Any nonsingular matrix has  $p$ th roots, and they can be classified into two groups, those that are functions of  $A$  and those that are not. We present a Schur algorithm for computing a matrix  $p$ th root that generalizes methods of Björck and Hammarling (1983) and Higham (1987) for the square root. Our algorithm forms a Schur decomposition of  $A$  and computes a  $p$ th roots of the (quasi)triangular factor by a recursion. The backward error associated with our Schur method is examined, and we find that the method has excellent numerical stability.

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*Multigrid methods for matrices with structure*

<sup>†</sup>**Jochen Staudacher & Thomas Huckle** (<sup>†</sup>Institut f. Informatik, Technische Universität München)

This talk will mainly be concerned with the 'Matrix Multilevel Method' which is based on a purely matrix dependent description of multigrid methods. I will motivate using a black box prolongation  $C$  by shifting the original matrix  $A$  in the form  $B = \alpha I - A$  and picking out every second column to  $C = B(:, 2 : 2 : n)$ . Here  $\alpha$  has to be chosen as a rough upper estimate of the largest eigenvalue of  $A$ . It will be pointed out how this originally one-dimensional approach can be carried over to separable - and even to more general - two-dimensional elliptic PDEs. The test results are very promising: I will give various numerical examples of elliptic PDEs with highly varying or discontinuous coefficients where standard multigrid deteriorates whereas the new method shows optimal behaviour. Clearly, the 'Matrix Multilevel Method' is more generally applicable than standard multigrid.

In the final part of the talk I will be concerned with the special case of multigrid methods for highly structured linear systems, in particular Toeplitz systems: Toeplitz systems and Block-Toeplitz systems with Toeplitz-Blocks are connected with generating functions whose coefficients are the entries of the matrix. Regarding prolongation and restriction also as Toeplitz matrices, a two-grid step can be analysed in terms of functions. Finally, - time permitting - an outlook to problems in image processing will be given.

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*n-widths for singularly perturbed problems*

<sup>†</sup>**Martin Stynes & R. Bruce Kellogg** (<sup>†</sup>National University of Ireland)

Kolmogorov  $n$ -widths are an approximation theory concept that, for a given problem, yields information about the optimal rate of convergence attainable by **any** nu-

merical method applied to that problem. We survey sharp bounds recently obtained for the  $n$ -widths of certain singularly perturbed convection-diffusion and reaction-diffusion problems.

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*Spectral methods for Third-order differential equations*

<sup>†</sup>**W. Sun** (<sup>†</sup>City University of Hong Kong)

In this talk, we present a Legendre Petrov-Galerkin method for a class of nonlinear third-order partial differential equations with non-periodic boundary conditions. This includes many popular cases, such as the well-known Korteweg-de Vries (KdV) equation, the modified KdV equation and nonlinear lattice equations, with a wide range of applications in physics and engineering. In our method, the nonlinear term is computed with the Legendre spectral method and some pseudospectral methods, respectively. Optimal error estimates in  $L_2$ -norm are obtained for both semi-discrete and fully discrete schemes. The methods are also applicable to some  $(2m + 1)$ th-order differential equations.

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*Multistep methods for fully nonlinear parabolic equations - how do they behave?*

<sup>†</sup>**M M Thalhammer & A Ostermann** (<sup>†</sup>University of Innsbruck)

We study multistep discretizations of fully nonlinear parabolic differential equations on a Banach space working in the analytical framework of sectorial operators and Hölder continuous functions. Our interest in such an abstract initial value problem is caused by the fact that various initial-boundary value problems describing nonlinear diffusion can be cast in this form.

We present convergence results and further study the qualitative behaviour of the time discretization over long times. For illustrating the theoretical results, numerical examples are presented.

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*Efficient methods for estimating eigenvalue spectra*

<sup>†</sup>**Ken Thomas, Simon Cox & Geoff Daniell** (<sup>†</sup>University of Southampton)

The eigenvalue problem is central to many applications in mathematical physics and numerical analysis. In this paper, we describe two methods for estimating the spectrum of a symmetric matrix  $A$  by calculating a density function. The density is derived from moments generated by matrix-vector products; that is from a Krylov sequence using the Chebyshev recurrence formula.

The first method extends the work of Lanczos (Lanczos 1957) who interpreted the moments as Fourier coefficients. By taking a sufficiently large number of moments, the detail in the spectrum can be as fine as desired.

The second method uses maximum entropy to select

the most probable density consistent with the moment data. The eigenvalue problem is reformulated as a reduced Hausdorff moment problem. (Skilling 1989) was the first to propose maximum entropy as a method for finding the spectrum of very large matrices. The major problem is that the Hausdorff moment problem is extremely ill-conditioned. The consequence is that there is a limit to the number of moments that can be used before the ill-conditioning prevents solution. On the other hand, it can give good reconstructions from few moments.

Our method has been intended to provide a useful tool in eigenvalue problems of very large matrices when the only feasible operation is matrix-vector multiplication. We can extend it to the generalised eigenvalue problem.

[1] Lanczos (1957). Applied analysis. London, Isaac Pitman.

[2] Skilling, J. (1989). The eigenvalues of mega-dimensional matrices. Maximum Entropy and Bayesian Methods, Kluwer Academic.

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#### *Bounds for Eigenvalues of Matrix Polynomials*

<sup>†</sup>**Françoise Tisseur & Nicholas J. Higham** (<sup>†</sup>University of Manchester)

Polynomial root finding is an old subject on which much has been written. When the coefficients of the polynomial are generalized from scalars to matrices we obtain the polynomial eigenvalue problem

$$P(\lambda)x = (\lambda^m A_m + \lambda^{m-1} A_{m-1} + \dots + A_0)x$$

where the  $A_i$  are complex matrices and  $\lambda$  is an eigenvalue with corresponding eigenvector  $x$ . To our knowledge little or nothing has been published on bounds for eigenvalues of matrix polynomials, except for special classes of coefficient matrices.

We derive upper and lower bounds for the absolute values of the eigenvalues of general matrix polynomials  $P(\lambda)$ , concentrating on bounds that are of practical use. Thus we aim for bounds that can be computed with much less computational effort than is required to solve the eigenproblem, especially for large problems. The bounds are based on norms of the coefficient matrices and involve the inverses of the leading and trailing coefficient matrices. They generalize various existing bounds for scalar polynomials and single matrices. A variety of tools are used in the derivations, including block companion matrices, Gershgorin's theorem, the numerical radius, and associated scalar polynomials. Numerical experiments show that the bounds can be surprisingly sharp on practical problems.

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#### *Large and infinite-dimensional optimization for systems governed by PDE*

<sup>†</sup>**Victor K. Tolstykh** (<sup>†</sup>Donetsk State University)

There is proposed a new interpretation of necessary condition for optimality (NCO) for unconstrained objective functional  $J(u)$  subject to partial differential equations (PDE) with control  $u$ . It can be optimal control problem, optimal design or parameter identification. NCO is written for a descent trajectory and not just for a stationary point:  $\frac{\nabla J(x; u^{k+1})}{\nabla J(x; u^k)} = \text{const}^k$ ,

where  $k$  denotes a point in a descent trajectory. NCO was implemented by optimization method:  $u^{k+1}(x) = u^k(x) - b^k \alpha^k(x) \nabla J(x; u^k)$ , where  $\alpha^k(x)$  is a function at  $k$ -iterate from NCO. The gradient  $\nabla J(x; u)$  is calculated by Lagrange multipliers techniques.

There are comparative computing tests for quadratic large and in infinite-dimensional problems with parabolic and hyperbolic PDE. There are Internet URLs at test software.

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#### *Spectral Differencing with a Twist*

<sup>†</sup>**Manfred R Trummer & Richard Baltensperger** (<sup>†</sup>Simon Fraser University)

Spectral collocation methods have become very useful in providing highly accurate solutions to differential equations. A straightforward implementation of these methods involves the use of spectral differentiation matrices. To obtain optimal accuracy these matrices must be computed carefully. We demonstrate that naive algorithms for computing these matrices suffer from severe loss of accuracy due to roundoff errors. Several improvements are analyzed and compared. A number of numerical examples are provided, demonstrating significant differences between the sensitivity of the forward problem and inverse problem.

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#### *Genetic Algorithms for Simulating Counting Behaviour.*

<sup>†</sup>**Scott Turner, R G M Crockett & P D Picton & E Triastuti** (<sup>†</sup>University College Northampton)

Under many circumstances, a data-set arising from a data-acquisition exercise will yield a spiky frequency distribution containing periodic structure where, under ideal circumstances, no such structure would have been present. Such periodic structure can contain a variety of periods and be short- or long-range.

Such structure in frequency distributions arises from the counting behaviour: such practices include those entailing rounding processes (e.g. rounding and estimation) and, possibly, falsification and the more individuals and processes present in the overall compilation, the greater the potential variety of practices.

In essence, where rounding processes occur, observations at inconvenient sizes are rounded either explicitly (rounding) or implicitly (estimation) to convenient sizes. In decimal systems, convenient sizes are commonly multiples of base-units such as 5 and 10, for example or, in duodecimal systems, multiples of

6 (half-dozen) and 12 (dozen), for example. Consequently, rounding processes yield excesses of convenient numbers: those numbers having a regular, periodic spacing within the range of sizes observed.

Falsification takes a wide variety of forms the intent under these circumstances, after all, is to deceive and so the type of structure encountered as a result of falsification is potentially more complex than that arising due to rounding processes.

We have constructed two implementations of Genetic Algorithms which simulate counting behaviour i.e. the combination of practices utilised in the compilation of a (numerical) data-set. One implementation can be regarded as a forward algorithm, imposing structure onto an idealised source sample with the recorded spiky data as target. The other can be regarded as a reverse algorithm, basically removing structure from the recorded data to produce an idealised smooth frequency distribution. In both implementations, the algorithms record their activity on an observation-by-observation basis, providing a quantification of the structure present in a data-set in terms of both overall extent and the bases to which observations are rounded.

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*Optimal implicit exponentially-fitted Runge-Kutta methods*

†**Guido Vanden Berghe** (†Ghent University)

Implicit Runge-Kutta methods for first-order ODEs are considered and the problem of how frequencies should be tuned in order to obtain the maximal benefit from the exponential fitted versions of such algorithms is examined. The key to the answer lies in the analysis of the behaviour of the error. A two-stage implicit Runge-Kutta method is particularly investigated. Formulae for optimal frequencies are produced; in that case the order of the method is increased by one unit. A numerical experiment illustrates the properties of the developed algorithms.

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*Phase Space/Stability Error Control for Dynamical Systems*

†**R. Vignesvaran, A.R. Humphries & N. Christodoulou** (†Eatern University (visiting University of Sussex))

We consider a phase space/stability error control for numerical simulation of dynamical systems. We illustrate how variable time-stepping algorithms perform badly for long time computations which pass close to a fixed point. A new error control is introduced in which the local truncation error at each step is bounded by a fraction of the solution arc-length over the corresponding time interval. We show how this control can be thought of as either a phase space or a stability control. We introduce a step-size selection scheme which allows this error control to be incorporated within the

standard adaptive algorithm as an extra constraint at negligible extra computational cost. Numerical and theoretical results are presented to illustrate the behaviour of this new method. For linear systems with a stable hyperbolic fixed point, this error control gives a numerical solution which is forced to converge to the fixed point. We also consider the dynamics in the neighbourhood of saddle points.

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*Periodic Orbits of the N-body Problem*

†**Divakar Viswanath** (†University of Chicago)

I will describe an algorithm to compute periodic orbits of the N-body problem. The algorithm is based on Fourier series and uses three components:

- \* a descent direction, which is found in a manner similar to the derivation of the Euler-Lagrange equations from the Lagrangian in classical mechanics,
- \* a Newton step, which uses the Lindstedt-Poincare method in perturbation theory, and
- \* imposition of constraints to respect the symmetries of the Hamiltonian.

The three components are glued together using Powell's dogleg strategy, devised for trust region methods in unconstrained optimization, to obtain a highly convergent and accurate algorithm. I will show accurate computations of several remarkable periodic orbits discovered by the physicist Cristopher Moore and some other examples.

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*Incremental Norm Estimation for Dense and Sparse Matrices*

†**Christof Voemel & Iain S. Duff** (†CERFACS)

We discuss the benefits of an incremental approach to norm estimation for triangular matrices. Our investigation covers both dense and sparse matrices. If we use our incremental norm estimation on explicitly generated entries of the inverse of the triangular matrix, we can relate our results to incremental condition estimation (ICE). We show that our algorithm extends more naturally to the sparse case than ICE. Our scheme can be used to develop a robust pivot selection criterion for QR factorization or as the basis of a rank-revealing factorization.

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*Moving boundary problems from materials science*

†**C. Vuik, W. van Til, F.J. Vermolen & S. van der Zwaag** (†Delft University of Technology)

As-cast aluminium alloys often contain particles and other inhomogeneities, which deteriorate the mechanical properties both for further processing and final use. These inhomogeneities can be removed with a thermal treatment, during which the metallurgical state of the material changes. These changes can either involve the dissolution or morphology of the various phases. A mathematical model is proposed to describe dis-

solution of multi-component particles. In this model equations are given to determine the position of the particle boundary in time, using a number of diffusion equations which are coupled by nonlinear boundary conditions at the interface. This problem is known as a vector valued Stefan problem.

A numerical method is described to solve a vector valued Stefan problem for one space dimension. From an asymptotic analysis it appears that the solution can also be approximated with a scalar Stefan problem where the diffusion coefficient and concentrations are replaced by their weighted averages. A comparison of both approaches is given.

Recently we also started to study morphology changes of the various phases. We consider the transformation of plate-shaped particles (  $\text{Al}_5\text{FeSi}$  ) into spherical-shaped particles (  $\text{Al}_{12}\text{Fe}_3\text{Si}$  ). For this problem two or three dimensional configurations are required. A mathematical model, as well as some numerical results are presented.

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*The Riccati Trail*

<sup>†</sup>**Eugene L Wachspress** (<sup>†</sup>)

The quest for the solution  $X$  of the Riccati matrix equation  $AX + XA^T + FX = C$ , motivated analysis leading to a sequence of innovative numerical methods which have been implemented with student MATLAB. Newton iteration on the nonlinearity requires solution during the  $t$ -th step of the Lyapunov matrix equation  $A[X]X_t + X_t A[X]^T = C[X]$ , where  $A[X] = A + FX_{t-1}$  and  $C[X] = C + FX_{t-1}F$ . Matrix  $A[X]$  is reduced to a banded upper Hessenberg matrix  $S$ , with a sequence of Gaussian similarity transformations which yields a transformed equation  $SY + YS^T = C_S$ . Then eigenvalues on the spectral boundary of  $S$  are computed with shifted inverse iteration and deflation. These are used to compute efficient Alternating Direction Implicit (ADI) parameters. The reduced Lyapunov equation is solved with ADI iteration and  $Y$  is back transformed to give  $X_t$  for the next Newton iteration. The Gaussian reduction, eigenvalue computation, and ADI iteration for complex spectra all required extensive new analysis. ADI solution of similarly reduced Sylvester equations,  $AX + XB = C$ , required generalizations of two-variable ADI theory from the real to the complex domain. New methods were devised for solving Lyapunov and Sylvester equations with low order right hand sides.

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*Moving grid finite element methods for some pattern formation problems in biology*

<sup>†</sup>**Andy Wathen, Anotida Madzvamuse & Philip Maini** (<sup>†</sup>Oxford University)

We will describe the application of finite element techniques to the solution of certain reaction-diffusion PDEs

which are hypothesised to model/mimic pattern formation through the ‘Turing instability’ mechanism. For growing organisms, continuously expanding computational domains are employed and the finite element solution is computed on a correspondingly deforming grid.

We will show results on simple geometric shapes and also our computed patterns for a family of common butterflies both on static and growing domains.

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*Implicit Surface Fitting using Directional Constraints*

<sup>†</sup>**G A Watson, M Gulliksson & I Söderkvist** (<sup>†</sup>University of Dundee)

A commonly used technique for fitting curves and surfaces to measured data is that known as orthogonal distance regression, where the sum of squares of orthogonal distances from the data points to the surface is minimized. An alternative has recently been proposed for curves and surfaces which are parametrically defined, which minimizes the sum of squares in given directions which depend on the measuring process. In addition to taking account of that process, it is claimed that this technique has the advantage of complying with traditional fixed-regressor assumptions, enabling standard inference theory to apply. Here we consider extending this idea to curves and surfaces where the only assumption made is that there is an implicit formulation. Numerical results are given to illustrate the algorithmic performance.

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*Numerical computation of complex singularities in nonlinear PDEs*

<sup>†</sup>**J.A.C. Weideman** (<sup>†</sup>University of Stellenbosch)

Many nonlinear PDEs have solutions that become singular in finite time. Examples are the inviscid Burgers equation,

$$u_t + uu_x = 0,$$

and the nonlinear heat equation,

$$u_t - u_{xx} + u^2 = 0.$$

The first equation exhibits shocks and the second a pole-type blow-up. A less familiar example that also displays blow-up is

$$u_t + (H(u)u)_x - \nu u_{xx} = 0,$$

where  $\nu$  is a positive constant and  $H$  the Hilbert transform. (The equation has been proposed in connection with vortex sheet motion.)

In the last decade or two, it has been recognized that the analytic structure of the solutions  $u(x + iy, t)$  in the complex plane may aid in the understanding of the formation of singularities. D. Bessis and J.D. Fournier, for example, have studied the complex singularities corresponding to a special initial condition,

and determined the associated Riemann surface (*J. Physique Lett.* **45**, L-833, 1984). A similar study of the pole dynamics of () was reported by G.R. Baker et. al. (*Physica D* **91**, 349, 1996).

The singularity structure corresponding to general initial conditions or more complicated PDEs, including the 3rd above, may not be analytically tractable. The question arises how this may be computed numerically.

Here we propose a two-step strategy: The first step is the numerical solution of the PDE using a Fourier spectral method; the second step is numerical analytical continuation into the complex plane using the  $\epsilon$ -algorithm to sum the Fourier series. Numerical results involving equations above are presented.

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*Geometric integration methods for nonlinear diffusion equations.*

**†J F Williams & C J Budd** (†University of Bath)

In this paper geometric integration methods are applied to the nonlinear diffusion equation with extinction

$$u_t = \frac{1}{m} \nabla^2(u^m) - \beta u^q$$

where  $\nabla^2$  is the radial Laplacian in arbitrary dimension,  $m > 1$  and  $\beta \geq 0$ . This equation models several important physical processes and has the feature of being invariant under changes of scale. Singular solutions exist which may have interfaces or go to zero in a finite time. By considering the asymptotic solutions, scale-invariant moving mesh methods are constructed which have the same scaling invariance properties as the original equation. These methods use equidistribution of the spatial mesh based on the monitor function

$$M = |v_{xx}|^p$$

$v$  is the so-called pressure,  $v = u^{m-1}/(m-1)$ . We show that this formulation permits the accurate resolution of interfaces between regions where the solution is large and where it is small. And we consider the effects of the solution scaling on such issues as accuracy, stability and stiffness.

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*Algorithms for Rectangular, Generalised, Sparse and/or Weighted Pseudospectra*

**†Tom Wright & Nick Trefethen** (†Oxford University)

Ten years ago, pseudospectra had been computed of matrices of dimensions  $N \leq 32$ . Since then, improved algorithms have increased  $N$  as high as  $10^3$  for dense matrices and  $10^6$  for sparse matrices.

As this field matures, other kinds of algorithmic developments are also occurring. We will discuss three variations on the straightforward (grid based) pseudospectra computation:

\* weighted norms,

\* rectangular matrices,

\* generalised eigenvalue problems.

We have developed a system of algorithms that handle most of these features, and their combinations, accurately and fast. We will present a decision tree showing all the possibilities and focus on a few of particular applied or algorithmic interest.

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*Practical general linear methods*

**†Will Wright** (†University of Auckland)

When solving an ordinary differential equation numerically almost always a Runge-Kutta or a linear multistep method will be used. However, both of these traditional methods have well known disadvantages.

To express these traditional methods in a unifying framework, general linear methods were formulated by Butcher in 1965. However, identifying practical methods from this large class has proved difficult. Until recently general linear methods which were neither Runge-Kutta or linear multistep methods were found on a case by case basis. Furthermore, classes of methods which were not slight modifications of the traditional methods were not known.

A review of general linear methods will be presented, with particular emphasis on the identification of practical methods. One such class of methods, with a property known as “inherent Runge-Kutta stability” will be described. These methods are useful for the solution of stiff and non-stiff differential equations.

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*High Order Integration Formula Using Trigonometric Polynomials For Periodic IVPs*

**†Abdul Razak Bin Yaakub** (†Universiti Utara Malaysia)

In this paper a new fifth order Runge-Kutta type method for solving oscillatory problems by the use of trigonometric polynomials is proposed which extends the earlier work of Gautschi (1961). An analysis of the convergence and stability of the new method is given with comparison with the standard Runge-Kutta methods. Finally numerical results are presented which confirm the accuracy of the high order method.

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*New Fast Algorithms for Evaluation of Chebyshev Series on massive points in Numerical PDE Applications with Spectral Method*

**†Zhang Li Lun & Song JunQiang** (†ChangSha Institute of Technology)

The evaluation of orthonormal polynomials series is a basic procedure in PDE applications with spectral method. Chebyshev spectral method is the most popular one. Thus to evaluate Chebyshev series quickly as possible is important.

Two brand new algorithms for evaluation of Chebyshev series are given here. One is named “fast trans-

forming method”, which transforms the procedure into a simpler one of a common polynomial. The other is the direct improvement of the traditional ones of 1950’s, and the new algorithm can fully utilize the symmetry of discrete points. In short, the two new algorithms in this paper are both efficient compared with the traditional ones. For example, when the number of points is equal to the number of terms in the series, both methods can save at least half of the whole complexity.

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*Global search for starting point of local descent*

**†Antanas Zilinskas, A Jakaitiene & E S Fraga**

(†University College London)

Many applied optimization problems are formulated as black box or semi-black box optimization: unimodality of the theoretical model is not clear, but local descent algorithms practically stick at different points depending of the starting point. Optimizing chemical process designs is an example of such a problem. Chemical plant design models are nonlinear, nonconvex and discontinuous. When process heat integration is included through the use of stochastic methods for heat exchanger network synthesis, the chemical plant design model exhibits noise. A choice of an appropriate starting point for such problems is crucial. Several practical problems, including chemical process design, are analysed, characteristic cases are specified and recommendations for the global search of an appropriate starting point are discussed.