LMS Durham Symposium on Evolutionary Problems: Continuous and Discretized Nonlinear Systems 4-14th July 1992

Convener: Professor C.T.H. Baker (The Victoria University of Manchester)
Secretary to the Organising Committee:
Dr. Ruth Thomas (University of Manchester Institute of Science and Technology)
Supported in part by the UK SERC

TIMETABLE

Saturday 4th July

1430-1825	Registration
1845	Sherry reception (Grey College)
1915	Dinner (Grey College)

Academic programme: There appears below what is intended (barring 'force majeur') to be the final programme. **It is intended that participants make their own *ad hoc* arrangements for individual and joint research and working/discussion meetings, bearing in mind the programme and the interests of those involved.** (Where appropriate, information on meetings arranged should be posted by participants on the symposium noticeboards.) To assist, a list of attendance dates notified to us by participants (including changes up to 28-6-92) is available.

*The names supplied are those of the speakers; co-authors appear in the separate abstracts.

Sunday 5th July

0855-0900	C.T.H.Baker	Welcoming remarks
0900-1000	J.C.Butcher(1)	Runge-Kutta methods made difficult
1000-1030	**Coffee Break**	
1030-1130	V. Kolmanovskii	Stability of functional-differential equations and their applications
1130-1230	C. Elliott (1)	Curvature dependent phase boundary motion
1300	**Lunch**	
1400-1500	N.Trefethen(1)	Non-normality and its influence on continuous and discrete processes 1-an annotated history of spectral ideas
1500-1600	C. Grebogi	Numerical trajectories of chaotic systems
1600-1630	**Late Tea break**	
1630-1730	J.M. Sanz-Serna(1)	Numerical Hamiltonian Dynamics 1
1730-1830	M. Spijker	On numerical ranges and stability estimates
1900	**Dinner**	
2015-2115	A. Feldstein	Bifurcation and stability of a finite-dimensional smooth iterative map

Monday 6th July

0900-1000	J.Ockendon	The evolution of singularities in the Hele-Shaw free boundary problem
1000-1030	**Coffee Break**	
1030-1130	A.Iserles	On the pantograph equation and its generalizations
1130-1230	W. Enright	Continuous methods for DDEs, BVPs and DAEs
1300	**Lunch**	
1355-1410	Conference photograph:	Please assemble promptly at 1355 - Grey College steps
1410-1540		(i) Collaborative and individual research (ii) Mini-Symposium on: Volterra and Delay Equations and the Pantograph Equation (A. Iserles and C.T.H. Baker)
1540-1600	**Slightly late Tea break**	
1600-1630	D.Kershaw	Belt'jukov Runge Kutta methods for Abel Volterra integral equations
1630-1700	M.Buhmann*	Stability of the discretized pantograph differential equation
1700-1745	G. Derfel	On functional-differential equations with linearly transformed arguments
1745-1830	K. Wright	Differential equations for the analytic singular-value decomposition, and their solution
1900	**Dinner**	
2015-2100	Xinfu Chen,	Hele-Shaw problem and area-preserved curve-shortening motion
2100-2130	P Sharp (2) *	A class of variable step explicit Nordsieck multivalue methods

Tuesday 7th July

0900-1000	J.M. Sanz-Serna(2)	Numerical Hamiltonian Dynamics 2
1000-1030	**Coffee Break**	
1030-1130	R.D. Skeel	Canonical integration methods for molecular dynamics
1130-1230	J.Norbury	Weather forecasting and a Hamiltonian dynamical system
1300	**Lunch**	
1400-1530		(i) Collaborative and individual research (ii) Mini-Symposium on: Numerical Hamiltonian ODEs and Industrial Mathematics (R D Skeel and A K Parrott)
1530-1600	**Tea break**	
1600-1630	C. Paul*	An algorithm for the numerical solution of singular DDEs
1630-1700	J. Terjeki,	Stability and asymptotic stability for nonlinear pantograph equations
1700-1730	B. Leimkuhler	Numerical methods for constrained Hamiltonian systems
1730-1800	A.A. Sagle*	Critical elements of quadratic systems and algebras
1900	**Dinner**	
2015-2115	C. Budd	Spectral methods for a parabolic equation with blow-up

Wednesday 8th July

0900-1000	Y. Tourigny*	Decipherment of singularities by discrete variable methods.
1000-1030	**Coffee Break**	
1030-1130	A.Stuart	Dynamics of local error control mechanisms for dissipative and related dynamical systems
1130-1230	D.Higham	Steady states of adaptive time stepping algorithms
1300	**Lunch**	
1400-1530		(i) Collaborative and individual research (ii) Mini-Symposium on: Runge-Kutta (D.Kershaw)
1530-1600	**Tea break**	
1600-1630	Bai Fengshan*	Numerical method for dynamical phase transitions
1630-1700	J Williams*	Parameter estimation and approximation in ode's
1700-1730	D. Willé*	Towards an alternative error control strategy for ordinary and delay-differential equations
1730-1800	Karel in't Hout	Runge-Kutta methods in the numerical solution of delay-differential equations
1800-1830	M. Sofroniou	Symplectic integration schemes for general Hamiltonians to any order
1900	**Dinner**	
2015-2100	R. Vermiglio* L. Torelli*	Stability of some test equations with delay -parts 1 & 2
2100-2130	E Russo*	Block methods & V_0-stable methods for second-kind Volterra equations

Thursday 9th July

0900-1000	S. Larsson	Uniform long time error bounds for semi-linear parabolic equations
1000-1030	**Coffee Break**	
1030-1130	C. Elliott(2)	Global dynamics of discrete semilinear parabolic systems
1130-1230	J. Blowey*	Curvature dependent phase boundary motion: numerical simulations
1300	**Lunch**	
1400-1530	†	Collaborative and individual research
1530-1600	**Tea break**	
1600-1630	D. French	Analysis and computation of solutions to an evolution problem in nonlinear viscoelasticity
1630-1700	A. Hill	The approximation of attractors in a Banach space
1700-1730	B. Lu*	Mathematical and numerical analysis for the Dynamics Ising Model
1730-1800	Tang Qi	Contact problems in dynamical thermo-elasticity
1800-1830	S. McKee (1)	Integral inequalities and their application to numerical analysis
1900	**Dinner**	
2015-2115	B.D. Sleeman	The dynamics of reversible systems and and spatio-temporal complexity in biology

Friday 10th July

0900-1000	H.B.Keller*	The stabilization of unstable schemes: computing unstable solution paths via time integration
1000-1030	**Coffee Break**	
1030-1130	A. Spence*	Numerical detection of Hopf bifurcations in large systems arising in fluid mechanics
1130-1230	W.J. Beyn	Numerical treatment of global bifurcations in dynamical systems
1300	**Lunch**	
1400-1530	†	Collaborative and individual research
1530-1600	**Tea break**	
1600-1645	P. Glendinning	Global bifurcation theory - new routes to chaos
1645-1730	G. Moore	Computation of invariant manifolds
1730-1815	L.N. Trefethen(2)	Non-normality and its influence on continuous and discrete processes 2: stability and convergence in numerical analysis
1900	**Dinner**	
2015-2045	A Champneys*	A novel homoclinic bifurcation in a Hamiltonian system
2045-2115	P. Sweby*	On spurious asymptotic numerical solutions of 2-by-2 systems of ode's

† *A tour of the City/Cathedral may be possible. The times will clash with minisymposia (9th and 10th July) and numbers are limited - participants should sign up in the symposium office (CM205) as early as possible.*

Saturday 11th July

0900-1000	T.F. Russell	Eulerian - Lagrangian localized adjoint methods for miscible and immiscible flow
1000-1030	**Coffee Break**	
1030-1130	D.M. Sloan (2)	Pseudospectral techniques for singular problems
1130-1230	E. Suli	The analysis of Lagrange-Galerkin methods for evolutionary problems
1300	**Lunch**	
1400-1530		(i) Collaborative and individual research (ii) Mini-Symposium on: Evolutionary and Nonlinear Galerkin Methods (K.W. Morton and E. Suli)
1530-1600	**Tea break**	
1600-1645	J.W. Barrett*	Finite element approximation of p-Laplacian and related problems
1645-1730	D. Estep	Adaptive finite-element methods for reaction diffusion problems
1730-1815	G. Lord	Complex Ginzburg-Landau equation - numerical schemes and absorbing sets
1900	**Dinner**	
2015-2045	P Sharp (1),	Some explicit multi-derivative Runge-Kutta pairs

Sunday 12th July

0900-1000	K. Burrage	Parallel methods for ODEs
1000-1030	**Coffee Break**	
1030-1130	P. van der Houwen	Implicit initial value problem solvers on parallel computers
1130-1230	A. Bellen	Parallel implementations of wave-form relaxation methods
1300	**Lunch**	
1400-1530		(i) Collaborative and individual research (ii) Mini-Symposium on: Parallelism in Numerical Methods (L. Freeman and C. Addison)
1530-1600	**Tea break**	
1600-1645	M. Zennaro	Wave-form relaxation iterative schemes and Runge-Kutta methods
1645-1730	Z. Jackiewicz* (2)	Contractivity of wave-form relaxation Runge-Kutta iterations & related limit methods for dissipative systems ... .
1730-1815	J.C. Butcher (2)	General linear methods made easy
1900	**Dinner**	
2015-2115	D Stoffer	Geometric properties & global error estimates for stiff ode. solvers

Monday 13th July

0900-1000	L.N. Trefethen(3)	Non-normality and its influence on continuous and discrete processes 3: the time evolution of shear flows and other physical applications
1000-1030	**Coffee Break**	
1030-1130	Z. Jackiewicz* (1)	General linear methods for ODEs
1130-1230	J.M.Sanz-Serna(3)	Numerical Hamiltonian Dynamics 3
1300	**Lunch**	
1400-1445	D.B. Duncan	High order accurate and isotropic schemes for the nonlinear Klein Gordon equation
1445-1530	R.F. Streater	The free-energy theorem
1530-1600	**Tea break**	
1600-1630	T. Tang	Hermite spectral method and scaling factor
1630-1700	A. Gardiner	The influence of dispersion on the inviscid Burgers equation
1700-1730	C.T.H.Baker	Hors D'Oeuvres - Nonlinearity and the importance of having a memory
19.00	**Sherry**	
19.30	**Conference Dinner**	**- Bar extension** until 12 midnight

Tuesday 14th July

0845-1100 Day of departure - a coach to the station will be available

Research aspects of the symposium

The symposium brought together (over 10 days) research workers in the study, numerical solution, and modelling, of evolutionary problems. The main themes were:

1. Volterra and delay equations (including the pantogragh equation);
2. Numerical solution of Hamiltonian systems;
3. Industrial mathematics and bio-mathematics (including Chemostat problems);
4. Runge-Kutta methods and parallelism in numerical methods;
5. Dissipative dynamical systems and dynamical phase transitions and general dynamical theories;
6. Bifurcation;
7. Evolutionary and nonlinear Galerkin methods.

Major advances in thinking were reported by, amongst others, Bellen, Beyn, Burrage, Butcher, Grebogi, Jackiewicz, Keller, Kolmanovskii, Larsson, Sanz-Serna, Spijker, Stuart, Trefethen, van der Houwen and Zennaro, from overseas. This selection perhaps reflects a dominance in numerical aspects, but always informed by practical considerations of correct modelling or of the computing environment and the Applied Mathematics/Numerical Analysis theme was maintained. Amongst the UK participants, the following acted as a focus for various interests: Addison, Baker, Budd, Elliott, Freeman, Iserles, Kershaw, Morton, Norbury, Ockendon, Parrott, Spence, Suli. Rather than single out individuals, we present abstracts for all presentations given as lectures or as poster sessions in an appendix.

The symposium provided an environment for intensive exchange of mathematical ideas, with little time for leisure. (This provided a challenge to participants who were less dedicated or had less stamina than the key organisers!!) The organisers were themselves engaged in scientific cooperation and in discussion groups and were aware that many participants were likewise occupied. The positive effect of such collaborative exchanges was endorsed by other participants. It was particularly useful to be able to receive participants from the former Soviet bloc.

There were some disappointments in the withdrawal of some overseas participants, but in the event the richness of the intellectual environment was maintained.

No formal symposium proceedings are envisaged, but participants have been invited to submit papers with a numerical analysis component to one of the journals for which the convener acts as an editor.

Titles and Abstracts for the 1992 LMS-SERC
Symposium on Continuous and Discretized
Evolutionary Problems

F. Bai (with A. Spence and A.M. Stuart): Numerical Methods for Dynamical Phase Transitions

Abstract

The Cahn-Hilliard equation with Neumann boundary condition, which is one of the dissipative PDEs arising in the modelling of phase transitions, is considered. As a result of the gradient structure it is known that, if all equilibria are hyperbolic, the global attractor comprises the set of equilibria and heteroclinic orbits connecting equilibria to one another. The PDE is approximated by a Galerkin spectral discretization to produce a system of ODEs. Analogous results to those holding for the PDE are proved for the ODEs - in particular the existence and structure of the global attractor.

Heteroclinic connections in the system of ODEs are computed using numerical continuation on the attractor. The methods employed allow the calculation of connecting orbits which are *unstable* as solutions of the initial value problem. Some basic numerical results are given to validate the numerical methods for the Chafee-Infante problem. Further numerical results are given for the Cahn-Hilliard equation; these illustrate the previously unknown structure of their global attractors and the nature of the heteroclinic connections.

C.T.H. Baker

Nonlinearity, and the Importance of having a Memory

Abstract

The dynamical behaviour of ordinary differential equations becomes interesting when nonlinearities are admitted. The interest becomes absorbing when one also admits problems with memory (delay - differential equations). We address briefly some of the points of interest.

C.T.H. Baker see also C.A.H. Paul (with C T H Baker) and D.R. Willé (with C.T.H.Baker)

J.F. Blowey (with C.M. Elliott): Curvature Dependent Phase Boundary Motion: Numerical Simulations

Abstract

Many physical problems involve curvature dependent phase boundary motion, for example coarsening in phase separation.

Using formal matched asymptotic expansions one may show that phase field models with order parameter solving an obstacle problem approximate curvature dependent phase boundary motion. Numerical simulations of surfaces evolving according to their mean curvature are to be presented.

C.J. Budd: Spectral Methods for a Parabolic PDE with Blow-up

Abstract

Spectral methods are effective for linear parabolic PDEs with smooth solutions. However nonlinear parabolic PDEs may develop singularities in a finite time. In such cases spectral methods can give misleading (& spurious) solutions. Indeed I shall present an example in which the underlying PDE blows up in a finite time but the spectral solution decays to zero for all initial data. The talk will demonstrate that it is the parity (ie. odd/even) of the number of spectral modes which affects whether the qualitative structure of the spectral solution is a good representation of the underlying problem or gives a spurious solution.

M.D. Buhmann (with A. Iserles): Stability of the Discretized Pantograph Differential Equation

Abstract

In this talk, we shall study discretizations of the general pantograph equation

$$y'(t) = ay(t) + by(\theta(t)) + cy'(\phi(t)),\ t \geq 0,\ y(0) = y_0$$

where a, b, c and y_0 are complex numbers and where θ and ϕ are strictly increasing functions on the non -negative reals with $\theta(0) = \phi(0)$ and $\theta(t) < t$, $\phi(t) < t$ for positive t. Our purpose is an analysis of the stability of the numerical solution with trapezoidal rule decretizations, and we will identify conditions on a, b, c and the stepsize which imply that the solution sequence $\{y_n\}_{n=0}^{\infty}$ is bounded or that it tends to zero algebraically, as a negative power of n.

J.W. Barrett (with W.B. Liu): Finite Element Approximation of the p-Laplacian and Related Problems

Abstract

In this talk we consider the continuous piecewise linear finite element approximation of the p-Laplacian: Given $p \in (1, \infty)$, f and g; find u such that

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

where $d = 1, 2$ or 3. For sufficiently regular solutions, which we show to be achievable for a subclass of data f, g and Ω, we prove optimal error bounds in the norm $W^{1,q}(\Omega)$; $q = p$ for $p < 2$ and $q \in [1, 2]$ for $p > 2$. We extend these results to (i) more general degenerate monotone quasilinear elliptic equations; (ii) interface problems, where for example the p in the p-Laplacian takes different values either side of a smooth surface contained inside Ω; and (iii) a non-Newtonian flow system, where the viscosity obeys the Carreau or power law. Finally, in line with the theme of this meeting, we discuss how these results extend to the corresponding degenerate parabolic problems.

* Supported by SERC research grant GR/F81255.

A. Bellen: Parallel Implementations of Waveform Relaxation Methods

Abstract

Waveform Relaxation schemes are suitable for decoupling large scale systems of ordinary (and algebraic) differential equations into subsystems. Whereas Jacobi iterations allow one to solve concurrently all the subsystems which are to be solved at each iteration, in Gauss-Seidel and SOR iterations the subsystems must be solved sequentially.

Since the use of Gauss-Seidel and SOR iterations can result in a dramatic reduction of the number of iterations, it is sometimes preferable to adopt these types of iterations and to exploit parallelism in the solution of each individual subsystem. We shall discuss the advantages and disadvantages of this approach.

A. Bellen: see also Z. Jackiewicz (with A.Bellen and M. Zennaro)

W.J. Beyn: Numerical Computation of Connecting Orbits in Dynamical Systems

Abstract

Global bifurcations in parameterized dynamical systems are associated with the birth or death of nonstationary invariant sets, such as periodic orbits, homoclinic orbits, invariant tori and strange attractors. In this talk we focus on bifurcations related to homoclinic orbits, e.g. the creation of periodic orbits near homoclinics, the emergence of homoclinic branches from local singularities of higher codimension and degeneracies on branches of homoclinics.

We analyse numerical methods for calculating these phenomena and discuss some open problems.

K. Burrage: Parallel Methods for Ordinary Differential Equations

Abstract

Considerable attention has recently been given to the development of efficient parallel methods for the numerical solution of differential equations. In this talk some of these recent developments are reviewed. The talk will focus on two different approaches, namely parallelism across the method (as typified by the block method approach) and parallelism across the system (as typified by waveform relaxation). However, special techniques for certain classes of problems will also be considered.

The development of the talk will focus on historical perspectives, but at the same time it will attempt to give a critical and impartial view on the proliferation of parallel methods that are being proposed currently.

K. Burrage: see also P.W. Sharp (with K. Burrage)

J.C. Butcher: Runge-Kutta Methods made Difficult

Abstract

A survey will be given of order, stability and other properties of both explicit and implicit Runge-Kutta methods. The lecture will include a simple proof of the order conditions. It will also include a discussion of the so-called Runge-Kutta space, a framework for analysing properties of more general classes of methods.

J.C. Butcher: General Linear Methods made Easy

Abstract

Because they include as special cases such widely used methods as Runge-Kutta and linear multistep, general linear methods have a natural role in theoretical analysis. By concentrating on some alternative special choices related to practical considerations, some new potentially useful methods have recently been identified. These methods, known as DIMSIMs, appear to have applications for both stiff and non-stiff problem types and for both conventional and parallel environments. The lecture will survey early work on these methods and will also discuss some recent results.

J.C. Butcher: see also Z.Jackiewicz (with J.C.Butcher)

A. Champneys (with A. Spence and J.F. Toland): A Novel Homoclinic Bifurcation in a Hamiltonian System

Abstract

An autonomous, reversible, fourth-order Hamiltonian system modelling an elastic strut is studied numerically. The existence of a unique, reversible homoclinic orbit to the origin has recently been proved by Amick and Toland for parameter values $p < -2$. We compute a path of this orbit as p increases, using standard continuation techniques incorporating a method (due to Beyn) of truncating to a finite time-interval with projection boundary conditions. It is found that, for $p \geq -2$, many homoclinic orbits bifurcate from the primary one. Only two of these orbits persist until $p = 2$, where the dynamics are governed by a certain normal form. An analysis is proposed to explain these numerical results.

Xinfu Chen: Hele-Shaw Problem and Area Preserved Curve Shortening Motion

Abstract

We prove existence, locally in time, of a solution of the following Hele-Shaw problem: Given a simply connected curve contained in a smooth bounded domain Ω, find the motion of the curve such that its normal velocity equals the jump of the normal derivatives of a function which is harmonic in the complement of the curve in Ω and whose boundary value on the curve equals its curvature. We show that this motion is a curve shortening motion which does not change the area of the region enclosed by the curve. In case Ω is the whole plane $\mathbf{R}^2$, we also show that if the initial curve is closed to an equilibrium, i.e. to a circle, then there exists a global solution and the global solution tends to some circle exponentially fast as time tends to infinity.

G. Derfel: On Functional-Differential Equations with Linearly Transformed Arguments

Abstract

Functional-differential equations of the form

$$\sum_{j=0}^{\ell}\sum_{k=0}^{m} a_{jk}y^{(k)}(\alpha_j x+\beta_j)=0 \qquad -\infty < x < \infty$$

$$a_{jk}\in \mathbf{C} \qquad \alpha_j(\neq 0,1), \beta_j \in \mathbf{R}$$

are considered. Asymptotic behaviour of the solutions, and the existence of analytic, almost periodic compactly supported solutions will be discussed. Applications in probability theory and in the spectral theory of 'difference Shrödinger operators' will be given, also.

D.B. Duncan: High Order Accurate and Isotropic Schemes for the Non-linear Klein-Gordon Equation.

Abstract

We examine high order accurate and isotropic difference schemes for the non-linear Klein-Gordon equation which are based on compact difference operators in space coupled with both simple and symplectic time stepping. We give various examples and investigate energy conservation and the effects of mesh orientation on the solutions.

M.R. Crisci (with P.J. van der Houwen, E. Russo and A. Vecchio): Block Methods and V-Stable Methods for Second Kind Volterra Integral Equations

Abstract

In this paper we are concerned with the construction of highly stable methods for the numerical solution of the second kind Volterra integral equation:

$$y(t)=g(t)+\int_{t_0}^{t} K(t,s,y(s))ds \qquad t_0\le t\le T \tag{1}$$

The stability of the methods is tested with respect to the convolution test equation:

$$y(t)=1+\int_0^t[\lambda+\mu(t-s)]y(s)ds \qquad \mathrm{Re}(\lambda)\le 0 \qquad \mu<0 \tag{2}$$

The construction of the methods has been developed following two approaches.

In the first approach we introduce the block versions of Volterra linear multistep methods for integrating (1) on parallel computers. To this purpose let us define the k-dimensional block vector $y_{n+1}=(y_{ni})^T \quad i=1,\dots,k$ where y_{ni} denotes a numerical approximation to the exact solution values $y(t_n+c_ih)$.

The block method we introduce has the following expression:

$$Y_{n+1}=AY_n+BF^*(t_ne+h\theta,t_nc+ha)+hCk(t_ne+hb_1,t_{n-1}e+hc,Y_n) \tag{3}$$
$$+hDk(t_ne+hb_2,t_ne+hc,Y_{n+1})$$

where $F^*(t,s)$ is an approximation of the lag term function:

$$F(t,s)=g(t)+\int_0^s k(t,x,y(x))dx$$

θ, b_i, a, c are k-dimensional parameter vectors and A, B, C, and D are k-by-k matrices.

We choose D as a diagonal matrix, so that the method is suitable for use on parallel systems with k processors.

We have derived the order conditions and the stability matrix for the methods (3).

A first method ($k=2$) has been constructed; it has order 2 and it is *almost* V_0-stable. The construction of methods for $k>2$ is under consideration.

The second approach we consider consists in transforming (1) to a system of special Volterra equations and in applying an A-stable method to this system. The resulting method will be called the *transformed* method.

This approach works for any kernel $k(t,s,y)$ that can split according to

$$k(t,s,y)=k_1(t,s,y)+k_2(t,s.y)-k_2(s,s.y) \tag{4}$$

where the derivative of $k_2(t,s,y)$ with respect to t exists and where k_1 does not identically vanish for $t=s$. We prove that every transformed method arising from an A-stable method is V-stable.

Since A-stable methods of any order are available we can obtain for kernels of kind (4) V-stable methods of any order.

W. Enright: Continuous Numerical Methods for DDEs, BVPs and DAEs.

Abstract

New Directions in Software for ODEs — BVPs, DAEs and DDEs.

In recent years much work has been done on the development of reliable and efficient continuous numerical methods for IVP problems in ODEs. In this talk I will discuss how these ideas lead to new and effective approaches for the numerical solution of BVPs, DAEs and DDEs in ODEs. Ongoing work at the University of Toronto will be discussed and the possible gains in efficiency and reliability quantified.

D. Estep: Adaptive Finite Element Methods for Reaction - Diffusion Problems

Abstract

First I will present some experiments which suggest the need for fully adaptive schemes for singularly-perturbed reaction-diffusion problems. Next I will describe an approach to mesh adaption in space-time finite elements based on *a posteriori* error analysis. I will describe several general purpose codes for scalar and parallel machines which implement our adaptive error control and present some numerical examples.

A. Feldstein (with Z. Jackiewicz and Y. Kuang): Unstable neutral and delay "test" equations

Abstract

The linear equation

$$(*) \qquad y'(t) = A(t) + \sum_{i=1}^{M} B_i y(\beta_i(t)) + \sum_{i=1}^{N} C_i y'(\gamma_i(t))$$

is considered as a possible "test" equation for numerical stability studies of delay and neutral equations. When $\beta_i(t)$ and $\gamma_i(t)$ are linear, conditions are established under which equation (*) is totally unsuitable as such a test equation because the solution $y(t)$ is strongly unstable in that it oscillates unboundedly as $t \longrightarrow \infty$. Under other conditions, equation (*) is useful as a test equation because $y(t) \longrightarrow 0$ as $t \longrightarrow \infty$.

C.M. Elliott: Curvature Dependent Phase Boundary Motion

Abstract

The evolution of a hypersurface with normal velocity given by the sum of its principal curvatures may be approximated by the solution of the Allen-Cahn equation $\varepsilon^2 u_t = \varepsilon^2 \Delta u + u - u^3$. Related problems arise in solidification where the evolving surface is a phase boundary. For example the Stefan problem with surface tension may be approximated by the so called 'phase field model'. In this talk we discuss the connections between 'phase field' equations and 'free boundary problems'.

C.M. Elliott (with A. Stuart): Global Dynamics of Discrete Semilinear Parabolic Equations

Abstract

A class of scalar semilinear parabolic equations possessing absorbing sets, a Lyapunov functional and a global attractor is considered. The gradient structure of the problem implies that, provided all steady states are isolated, solutions approach a steady state as $t \to \infty$. The dynamical properties of various finite difference and finite element schemes are analysed. The existence of absorbing sets, bounded independently of the mesh size, is proved for the numerical methods. Discrete Lyapunov functions are constructed to show that, under appropriate conditions on the mesh parameters, numerical orbits approach steady state solutions as discrete time increases.

C.M. Elliott see also **J.F.Blowey (with C.M. Elliott)**

C.M. Elliott see also **B.Lu (with C.M. Elliott)**

A. Gardiner:
The Influence of Dispersion on the Inviscid Burgers Equation

Abstract

It is firmly established that progressive wave solutions of the Korteweg-de-Vries ($K.d.V.$) equation do not converge to shock wave solutions of the inviscid Burgers Equation as $\varepsilon \to 0$. (Lax and Levermore, Venakides). Here we carry out a series of numerical experiments in an attempt to determine the type of solution obtained from the $K.d.V.$ equation for $0 < \varepsilon < E$, where E is sufficiently large to linearise the problem approximately. Particular emphasis is given to values of ε close to zero and in the ranges where solitons are present and where recurrence of the initial condition occurs.

P.A. Glendinning:
Global Bifurcation Theory: New Routes to Chaos

Abstract

The talk will give a brief introduction to global bifurcation theory and go on to describe new cascades of bifurcations to chaos. These bifurcations involve alternating period-doubling and homoclinic bifurcations leading to maps on the boundary of chaos having periods P_n with

$$P_{n+1} = 2P_n + (-1)^n.$$

These cascades occur in flows modelled by (twisted) Lorenz semi-flows. This new robust route to chaos can also be seen in a more general context in which it is one of uncountably many possible routes to chaos described by a subshift of finite type in renormalisation.

A.Feldstein (with A. Iserles and D. Levin):
Massively Parallel Algorithms for Embedded Delay Equations

Abstract

The delay differential equation

$$y'(t) = F(t, y(t), y(\theta(t))), \quad y(0) = y_0$$

can be embedded into an infinite ODE system. Two classes of numerical methods arise from this embedding. One is generated by iterating the delay function $Q(t)$. The other truncates the embedding and yields a special structure that can exploited on massively parallel computers.

A. Feldstein (with Y. I. Kim)
Bifurcation and Stability of a Finite-Dimensional Smooth Iterative Map

Abstract

A certain class of finite-dimensional smooth iterative maps with a real control parameter is investigated to study the stability and the possible bifurcations of their fixed points. This class includes those maps which would arise from delay differential equations. It is shown, by an appropriate change of variables, that the given map can be converted to an equivalent N−dimensional one. The construction of a k-fold composite map is outlined and the notion of a k-periodic fixed point of such a composite map is introduced. Algorithms for the numerical determination of such a fixed point are briefly described using a damped Newton's method. Numerical experiments and bifurcation diagrams are included which confirm the theory.

D.A. French:
Analysis and Computation of Solutions to an Evolution Problem in Nonlinear Viscoelasticity

Abstract

I will discuss the numerical approximation of an evolution problem modelling the deformations of a simple viscoelastic material with a nonconvex energy. If time permits I will sketch the proof of a Theorem that states that the approximate solution will converge to the true solution at an optimal rate. I will also discuss the results of some numerical computations.

C. Grebogi: Numerical Trajectories of Chaotic Systems

Abstract

Chaotic processes have the property that relatively small numerical errors tend to grow exponentially fast. In an iterated process, if errors double each iterate and numerical calculations have 48-bit (or 15- digit) accuracy, a true orbit through a point can be expected to have no correlation with a numerical orbit after 50 iterates. On the other hand, numerical studies often involve hundreds or thousands of iterates. One may therefore question the validity of such studies. A relevant result in this regard is that of Anosov and Bowen who showed that systems which are uniformly hyperbolic will have the shadowing property: a numerical (or noisy) orbit will stay close to (shadow) a true orbit for all time. Unfortunately, chaotic processes typically studied do not have the requisite uniform hyperbolicity, and the Anosov-Bowen result does not apply. I will report rigorous results for nonhyperbolic systems: *numerical orbits typically can be shadowed by true orbits for long time periods.*

D. Higham: Steady States of Adaptive Time Stepping Algorithms

Abstract

The talk will concern the behaviour of adaptive ODE algorithms on nonlinear ODEs. It is well known that constant stepsize implementations of popular ODE formulas may fail to reproduce the dynamics of the underlying ODE correctly. This talk will address the question of whether standard error control techniques can improve the long-time behaviour.

A.T. Hill: The Approximation of Attractors in a Banach Space

Abstract

We shall summarise three new results on the approximation of $\mathcal{A}$, the attractor of a dissipative semigroup $S(t)$ defined on a Banach space $\mathcal{X}$. This is an important area of theoretical analysis, which seeks to show that asymptotic computations give an accurate representation of the attractor of the underlying equation.

The first of our theorems gives general conditions under which subsequences of attractors of discrete semigroups S_k defined on finite-dimensional subspaces $\mathcal{X}_m$ of $\mathcal{X}$, converge in the Hausdorff metric (as sets) to a compact set, Λ, invariant under $S(t)$. (Λ here is not necessarily unique.) This result complements the work of Hale, Lin and Raugel, who show strong convergence to $\mathcal{A}$ in a half metric.

Our second result concerns attracting sets, as developed by Kloeden and Lorenz. Using an independent and simplified construction, we demonstrate strong Hausdorff metric convergence for attracting sets of the S_k to $\mathcal{A}$ under less restrictive conditions than have been specified previously.

Our final result concerns the temporally semidiscrete approximation by linear multistep methods of the attractor of the evolution operator of the autonomous parabolic equation

$$u_t + Au = F(u); F(u)(x) = f(x, u, \nabla u)$$

where A is the infinitesimal generator of an analytic semigroup on $\mathcal{X}$. Here, a $q-$step approximation gives rise to a semigroup, S_k, on $\mathcal{X}^q$. Provided that $|\arg\{\sigma(A - a_0 I)\}| < \alpha$ and that the method is strongly $A(\alpha)-$stable, we show that the discrete semigroup possesses an attractor in a neighbourhood of

$$\cup_{x \in \mathcal{A}} \{x\}^q.$$

This implies upper semicontinuity of this latter set with respect to the approximating attractors parameterised by k.

This work was supported by SERC.

K. in 't Hout: Runge-Kutta Methods in the Numerical Solution of Delay Differential Equations

Abstract

Runge-Kutta methods are easily adapted to initial value problems for delay differential equations. In order to enable the execution of a Runge-Kutta step in the case of such problems, one faces the approximation of a number of solution values at prescribed, retarded points. This can be done by applying an interpolation procedure to known approximations from foregoing Runge-Kutta steps. The choice of interpolation procedure constitutes the adaptation of a Runge-Kutta method to initial value problems for delay differential equations. In the stability analysis of these methods much attention has been given in the literature to the test equation

$$U'(t) = \lambda U(t) + \mu U(t - \tau)$$

($t \geq 0$), where λ, μ are given complex numbers and τ is a constant with $\tau > 0$. We shall investigate the relevance of the stability results obtained in the case of the above test equation, for more general delay differential equations by considering the equation

$$U'(t) = LU(t) + MU(t - \tau)$$

($t \geq 0$), where L, M are matrices of arbitrary order that are not necessarily simultaneously diagonalizable.

P.J. van der Houwen: Implicit Initial Value Problem Solvers on Parallel Computers

Abstract

Implicit step-by-step methods for solving, numerically, the initial-value problem $\{y' = f(y),\ y(0) = y_0\}$ usually lead to implicit relations of which the Jacobian matrix is of the special form $I - hM \otimes \partial f(y_n)/\partial y + O(h^2)$, where n is the step number and M is some matrix characterizing the step-by-step method. Approximating the Jacobian by $I - hM \otimes \partial f/\partial y$ and application of modified Newton iteration using this approximation requires the LU- decomposition of $I - hM \otimes \partial f/\partial y$. If s and d are the dimensions of M and the initial-value problem, respectively, then the LU-decomposition of $I - hM \otimes \partial f/\partial y$ is an $O(s^3d^3)$-process, which is extremely costly for large values of sd. We shall discuss parallel iteration methods for solving the implicit relations that exploit the special form of the Jacobian matrix. Their main characteristic is that each processor is required to compute LU-decompositions of matrices of dimension d, so that this part of the computational work is reduced by a factor s^3. However, unlike Newton-iteration, the parallel iteration methods do not possess the same linear stability properties as the original implicit step-by-step method. Analogous effects occur in the parallel iteration of step-by-step methods approximating initial-value problems for VIEs, VIDEs and DDEs. In this contribution, we will concentrate on the linear stability properties of parallel iterated step-by-step methods for solving a variety of initial-value problems.

P.J. van der Houwen: see also **M.R. Crisci (with P.J. van der Houwen, E. Russo and A. Vecchio)**

A. Iserles: On the Pantograph Equation and its Generalizations

Abstract

The pantograph equation reads

$$y'(t) = Ay(t) + By(qt) + Cy'(qt), \tag{5}$$

$$y(0) = y_0 \in \mathbb{C}^d, \tag{6}$$

where A, B, C are $d \times d$ complex matrices and $q \in (0, 1)$. It features in many applications, from analytic number theory and probability theory to astronomy, wavelets and electrical engineering.

The main purpose of this talk is to analyse properties – existence, well-posedness and asymptotic behaviour – of the equation, by employing a range of techniques from analytic function theory and harmonic analysis. In particular, it is demonstrated that the equation admits Dirichlet and Dirchlet – Taylor expansions, and this is useful in characterising its asymptotic behaviour. We focus inter alia on the behaviour along the stability boundary, where the form of the attractor is highly nontrivial.

The pantograph equation can be generalised in a number of ways. Thus, we debate existence and asymptotic features of the advanced equation with $q > 1$, as well as presenting preliminary results for the pantograph Riccati equation $y'(t) = by(t) + ay(qt)(1 - y(qt)), y(0) = y_0$.

A. Iserles: see also **M. Buhmann (with A.Iserles)** and **A. Feldstein (with A. Iserles and D. Levin)**

Z. Jackiewicz (with J.C. Butcher): General Linear Methods for ODEs

Abstract

We investigate some classes of general linear methods for ordinary differential equations with state order q and order q or $q+1$. Examples of such methods are constructed with stability function matching the A-acceptable generalised Padé approximations to the exponential function.

Z. Jackiewicz (with A. Bellen and M. Zennaro): Contractivity of Waveform Relaxation Runge-Kutta Iterations and Related Limit Methods for Dissipative Systems In the Maximum Norm

Abstract

We analyse contractivity properties of Runge-Kutta methods with suitable interpolation implemented using the waveform relaxation strategy, for systems of ordinary differential equations which are dissipative in the maximum norm. In general this type of implementation, which is quite appropriate in a parallel computing environment, turns out to improve the stability properties of Runge-Kutta methods. As a result of our analysis, a new class of methods different from Runge-Kutta methods but closely related to them is determined, which combine their high order of accuracy and unconditional contractivity in the maximum norm. This is known not to be possible for classical Runge-Kutta methods.

Z. Jackiewicz: see also A. Feldstein (with Z. Jackiewicz and Y. Kuang)

D. Kershaw: Bel'tjukov Runge Kutta Methods for Abel Volterra Integral Equations

Abstract

Classical Runge Kutta methods do not usually take into account the presence of singularities in the solution. When the forcing term is smooth Abel Volterra equations of the second kind have solutions with singularities at the origin. Using techniques based on the work of F. de Hoog and R. Weiss modifications are made to Bel'tjukov Runge Kutta methods to treat singular equations successfully when the kernel of the equation has a square root singularity.

H.B. Keller (with G.M. Shroff): Stabilization of Unstable Schemes: Computing Unstable Solution Paths via Time Integration

Abstract

An algorithm is developed to compute stable and unstable steady states of parameterized dynamical systems using an assumed given procedure for numerical integration of the time dependent equation. The scheme must become unstable as the steady states change from stable to unstable. We are able to use the initial blow up to determine a basis for the unstable subspace. Then we use Newton's method on the projection of the equilibrium equations into this subspace and we use the given time integration in the orthogonal complement. This procedure can be used to stabilize other procedures, not only time integrations, which become unstable as some parameter is varied. We also find that pseudo-arclength continuation procedures can be simplified by using only the projection of the tangent to the path in the unstable subspace. Thus, many large scale bifurcation problems for which Newton's method is prohibitively expensive can be made tractable by using this procedure. The key element which allows the stabilization to work most effectively is that the dimension of the unstable subspace should be small compared to the dimension of the problem space. However the basis for this subspace must be suitably maintained as continuation proceeds and the subspace changes.

V. Kolmanovskii: Stability of Functional Differential Equations and their Applications

Abstract

General methods of stability investigation of functional differential equations with arbitrary delays will be discussed. Applications in medicine, ecology and control theory will be given.

V. Kolmanovskii: see also L. Torelli and R.Vermiglio (with V. Kolmanovskii)

W.B.Liu: see J.W. Barrett (with W.B. Liu)

S. Larsson:
Long-time Behaviour of Finite Element Solutions of Semilinear Parabolic Problems

Abstract

Various results and techniques concerning the long-time behaviour of finite element solutions of semilinear parabolic problems are surveyed. Topics include: uniform long-time error bounds for exponentially stable solutions, convergence of attractors, approximation of phase portraits in the neighbourhood of an unstable hyperbolic stationary point. The importance of error bounds for solutions with low initial regularity is emphasized.

B. Leimkuhler:
Numerical Methods for Constrained Hamiltonian Systems

Abstract

A Hamiltonian system subject to smooth constraints can be viewed as a Hamiltonian system on a manifold. Numerical computations, however, must be performed in Euclidean space. In this paper transformations from "Hamiltonian differential-algebraic equations" to ODEs in Euclidean space are considered.

In the first part, canonical parameterizations or local charts are developed and it is shown how these can be computed in a practical framework. Hamiltonian "underlying ODEs" defined on the space in which the constraint manifold is embedded are then constructed. It is shown that certain formulations lead to a stable constraint-invariant while others lead to an unstable invariant. Projection techniques are considered. Numerical experiments illustrate the degree to which both constraint and symplectic invariants are preserved under the discretization of the various formulations.

G. Lord:
The Complex Ginzburg-Landau Equation: Numerical Schemes and Absorbing Sets

Abstract

Although it is well known that the complex Ginzburg-Landau equation defines a dynamical system, and that absorbing sets exist in both L^2 and H^1 which yield the existence of a global attractor, little or no attention has been paid to how the equation should be discretized in this context.

My aim in constructing numerical methods is to obtain a discrete dynamical system which has absorbing sets in the discrete L^2 and H^1 spaces which are bounded independently of initial data.

The method of analysis will be indicated and results presented for fixed step schemes.

B.Lu (with C.M. Elliott)

Mathematical and Numerical Analysis for the Dynamics Ising Model

Abstract

We consider the following mean-field equation of motion for the dynamic Ising model on a periodic lattice Λ:

$$\begin{cases} u_t + u = \tanh(\beta A u) & t > 0 \\ u(0) = u_0 & \\ u_{a+Ne_i} = u_a & a \epsilon \Lambda, 1 \leq i \leq d \end{cases}$$

where Λ denotes the lattice of $\mathbb{Z}^d$ with N^d sites defined by

$$\{a : a = \sum_{i=1}^{d} a_i e^i, a_i \epsilon \mathbb{Z}, 1 \leq a_i \leq N\}$$

with e^i being the standard unit vector of $\mathbb{Z}^d$. Here $u = (u_a)_{a \epsilon \Lambda}$ and u_a denotes the expectations of the spin at site a of the lattice. The $N^d \times N^d$ symmetric matrix A is defined by $\{Av\} := \sum_{b \epsilon \Lambda} E_{ab} v_b$ where $J_{ab} = J E_{ab} (J > 0)$ is the Ising interaction between sites a and b satisfying, for all $a, b \epsilon \Lambda$

(i). $E_{ab} \neq 0 \Longleftrightarrow \sum_{i=1}^{d} | a_i - bi | = 1$

(ii). $| E_{ab} | \leq 1$.

The parameter $\beta = J/\theta$, where $\theta (> 0)$ is the absolute temperature.

A Lyapunov functional shall be defined by

$$I(u) := \frac{1}{2} J h^2 (Lu, u) + (e, \psi(u))$$

where $(\cdot, \cdot)$ is the discrete weighted L^2 inner product $(u, v) = h^d \sum_{a \epsilon \Lambda} u_a v_a \ \forall u, v \epsilon V_\Lambda$, $\theta_c := J \max_{a \epsilon \Lambda} \sum_{b \epsilon N(a)} | E_{ab} |$, $L := -\frac{1}{h^2}(A - \frac{\theta_c}{J} I)$ and $\{e\}_a = 1, \forall a \epsilon \Lambda . \psi(r) := \frac{\theta}{2}((1+r) ln(1+r) + (1-r) ln(1-r)) - \frac{\theta_c}{2} r^2$.

A global attractor $B = \{u : \| u \|_\infty < 1\}$ is studied. The steady state solutions, dependent on the absolute temperature θ, are given. When $\theta > \theta_c$ then $\mathbf{0}$ is the unique equilibrium. When $\theta < \theta_c$, there exist at least three equilibria. The existence of and boundedness of absorbing sets are analysed. Moreover, various finite difference schemes such as the explicit Euler scheme and the predictor-corrector scheme and so on are constructed and their convergence, stability and dynamical properties are discussed. Finally, numerical examples are computed and analysed.

S. McKee

Integral Inequalities & their Application to Numerical Analysis

Abstract

Generalisations of the original Gronwall inequality abound. Discrete versions of these are fundamental to most convergence proofs. A general framework is constructed that permits the derivation of these inequalities in a natural way. Their application is illustrated using several Volterra integral and integro-differential equations arising from science and engineering.

G. Moore:

The Computation of Invariant Manifolds

Abstract

Most methods for calculating invariant manifolds of differential equations follow, directly or indirectly, solution trajectories on the manifold. We consider the manifold as a geometric object and wish to compute it independent of the dynamics of the underlying differential equation. Applications of the basic idea to periodic solutions, connecting orbit pairs and invariant tori will be presented.

D. Needham:

The Effects of Geometrical Spreading in Two and Three Dimensions on the Formation of Travelling Wave Fronts in a Simple Isothermal Chemical System

Abstract

In this paper we study the effects of geometrical spreading in two and three space dimensions on the formation of travelling chemical wavefronts for simple isothermal chemical systems. In particular we consider the case of cubic and quadratic autocatalysis, which were examined by Merkin and Needham and by Gray et al for the case of one-dimensional slab geometry. It is established that, in higher space dimensions, geometric effects alone may induce threshold phenomena which are not present in the one-dimensional case.

J. Norbury:
Weather Forecasting and a Hamiltonian Dynamical System

Abstract

An unusual Hamiltonian dynamical system with a discontinuous implicit global nonlinearity will be described, along with its solutions. This system has applications in weather forecasting.

J.R. Ockendon:
The Evolution of Singularities in the Hele-Shaw Free Boundary Problem

Abstract

In the absence of any regularising mechanism such as surface energy, the Hele-Shaw free boundary problem, which is a special case of the Stefan problem, almost always develops singularities in finite time. Indeed, when the free boundary is receding, the problem is ill-posed and it has proved impossible even to construct a weak solution beyond the first blow-up time (which would be zero if the initial data were not analytic). This talk will describe how conformal mapping can possibly shed some light on this situation.

J.R. Ockendon:
Some Reminiscences about the Physical Background of the Pantograph Equation

Abstract

Although the pantograph equation had been written down several decades earlier, there was an upsurge of interest in the 1970's following its use as a model for oscillations in railway overhead catenaries. This talk will recall the physical applicability of some of the early modelling and asymptotic and numerical analysis.

C. Paul (with C.T.H. Baker):
Stability Regions for $y'(t) = \lambda y(t) + \mu y(t-\tau)$

Abstract

In recent years, several codes for the numerical solution of *delay differential equations* have been developed. These codes have fuelled the interest in the stability of numerical methods for DDEs. Of particular interest is the stability of Runge-Kutta methods applied to the linear stability DDE

$$y'(t) = \lambda y(t) + \mu y(t-\tau),$$

where

$$\tau = (N+\vartheta)h \quad \text{for } 0 \le \vartheta \le 1 \text{ and } N \in \mathbb{Z}^+.$$

Although the stability equation is known, until now the stability regions that have been published for Runge-Kutta methods have been for $\lambda \in \mathbb{R}$ with $\mu \in \mathbb{C}$. This may be partly due to the fact that for λ and $\mu \in \mathbb{R}$, the standard boundary-locus technique often fails, in practice, to map out the whole of the stability region because, among other reasons, the partitioning loci describe unbounded paths.

First we describe a new method for mapping out disjoint stability regions. Then we present a selection of stability regions for varying N and ϑ for the *improved Euler method*, the *implicit trapezoidal method* and the *fifth-order Dormand and Prince method* with a fourth-order continuous embedded approximant and a fifth-order hermite approximant. The stability regions suggest that the size of the delay τ can drastically affect the stability of a Runge-Kutta method but that, as $\tau \to \infty$, the stability region can rapidly tend to its limiting form.

C. Paul (with C.T.H. Baker): An Algorithm for the Numerical Solution of Singular Delay Differential Equations

Abstract

An aspect of the development of Runge-Kutta codes for the numerical solution of a *delay differential equation* $y'(t) = f(t, y(t), y(t-\tau))$, $t \geq t_0, \tau \equiv \tau(t)$, is considered. The formulae require approximate derivative values that in turn use approximations to values of $y(t-\tau)$. In the case that $\tau \geq \gamma$ for all $t \geq t_0$ and for some constant γ, the easiest technique is to restrict the stepsize h so that $h \leq \gamma$; the approximations to $y(t-\tau)$ are then readily obtained from solution values computed at earlier steps. However, if τ is small relative to the stepsize, a method of evaluating the approximate value of $y(t-\tau)$ when $(t-\tau)$ lies in the current Runge-Kutta interval is desirable. In the case of *singular DDEs* $\tau(t_\alpha) = 0$, at one or more points $\{t_\alpha\}$ and such a process is then *necessary*. If $t_\alpha \neq t_0$, one possibility is to rely on extrapolation using the approximant from the last step; it is computationally cheap and easy to implement. However, because of the nature of singular points (the solution may be radically different beyond t_α, and clusters of derivative discontinuities may occur about t_α), extrapolation may not be suitable. Certainly, in the case of *initial value DDEs*, where $\tau(t_0) = t_0$, extrapolation is not possible (as no previous approximant exists).

One method for solving singular DDEs is due to Tavernini. In this talk a similar approach to Tavernini's is used to obtain a different method. The implementation of the method is presented, along with some theorems about its order and stability. As with Tavernini's method, the algorithm is also suitable for *Volterra functional equations*. Although computationally expensive, the algorithm has considerable scope for parallelization for ODEs, non-singular DDEs and singular DDEs. Some test problems are presented to evaluate the performance of the algorithm.

T.F. Russell: Eulerian-Lagrangian Localized Adjoint Methods for Miscible and Immiscible Flow

Abstract

Many fluid flows of practical interest, including miscible and immiscible flows in porous media, are often convection-dominated. Such problems contain parabolic and hyperbolic aspects, both of which need to be approximated efficiently and accurately. Standard approaches generally face a choice between numerical diffusion, nonphysical oscillations, and impractically fine grids. Schemes that combine Eulerian fixed-grid calculations of non-convective phenomena with Lagrangian characteristic treatment of convection, studied under a variety of names (characteristic Galerkin methods, modified method of characteristics, Eulerian-Lagrangian methods etc.), have overcome these limitations. Their principal drawbacks have been lack of mass conservation and the absence of a systematic formulation for general boundary conditions.

Eulerian-Lagrangian localized adjoint methods (ELLAM), based on space-time finite elements oriented along characteristics, fill these gaps. The speaker will present formulations, theoretical analyses, and numerical results for model problems of miscible and immiscible flow. Various portions of the talk are based on collaborations with H.K. Dahle, R.E. Ewing, R.M. Healy, R.V. Trujillo, and H. Wang.

A.A. Sagle (with M.K. Kinyon): Critical Elements of Quadratic Systems

Abstract

Quadratic systems such as the Lorenz equation, Euler equation, predator-prey model may be studied by expressing them as a quadratic system $X' = X^2$ occuring in an algebra A. The scope of quadratic systems is very wide as the solution of an autonomous polynomial differential equation may be given by a quadratic system. The use of algebras to study quadratic systems was initiated by L. Markus with the theme that the structure of algebras helps determine the behaviour of solutions. We apply this idea to the critical elements, i.e. the equilibrium and periodic solution of $X' = X^2$ in A. Thus an equilibrium solution N satisfies $N^2 = 0$, i.e. a nilpotent element, and idempotent elements $P = P^2$ determine their stability. In case idempotents do not exist, a Lyapunov function naturally defined by the algebra may be used. The automorphisms of the algebra help determine the domains of attraction and give explicit solutions for periodic orbits. We determine the 3-dimensional algebras for which solutions are given by automorphisms, and note that these solutions determine a cone which is almost an attractor.

J.M. Sanz-Serna: Numerical Hamiltonian Dynamics

Abstract

Physical phenomena where dissipation is negligible may always be modelled by systems of (ordinary or partial) differential equations of Hamiltonian form. The flow of a Hamiltonian system can be told apart from the flow of a non-Hamiltonian

system through the property of symplecticness, i.e. by the conservation of the Poincaré invariants. All qualitative properties specific to Hamiltonian systems derive from the symplectic property of the associated flows.

When Hamiltonian systems are solved numerically by standard techniques such as explicit Runge-Kutta methods, the map that advances the solution turns out not to be symplectic and hence is qualitatively wrong. The recent literature has devoted some effort to the construction of numerical methods that, when applied to Hamiltonian systems, inherit the property of symplecticness. In the talks I shall study these so-called symplectic methods. I shall in turn consider the questions (i) What is symplecticness? (ii) What symplectic numerical methods are known? (iii) Why should symplectic methods be expected to be better than standard methods? (iv) Are symplectic methods any better in practice than standard methods?

P.W. Sharp: Some Explicit Multiderivative Runge-Kutta Pairs

Abstract

Explicit Runge-Kutta formulae are often used to solve non-stiff first order initial value problems. It is well known that at least six stages are required to form an order five formula, if all the stages are evaluations of the first derivative. However, if one stage is an evaluation of the second derivative, only five stages are needed.

We derive and test a class of (4,5) explicit multiderivative Runge-Kutta pairs in which the second stage is an evaluation of the second derivative. The order five formula has five stages, while the order four formula has six stages. The sixth stage is re-used as the first stage of the next step, which means the new pairs require only five evaluations per step. Our numerical tests show, for both exact and finite difference second derivatives, that representative pairs from the new class are of comparable efficiency to explicit Runge-Kutta (4,5) pairs.

P.W. Sharp (with K. Burrage): A Class of Variable Step Explicit Nordsieck Multivalue Methods

Abstract

Existing integrators for non-stiff initial value problems often use Adams, Runge-Kutta or extrapolation methods. Few integrators based on explicit multivalue methods have been developed, even though their generality can potentially lead to improved performance.

We derive, search and test a class of variable-step, three-step, three-stage, explicit Nordsieck multivalue methods of order six. The methods use the order six formula to advance approximations to the solution and scaled first derivatives from the previous three steps. An embedded order five formula is used to form the local error estimate. The methods have stage order five which enables us to construct a local continuous extension of order five without performing extra derivative evaluations.

Our numerical results show, despite the simplicity of our implementation, that the new methods are competitive with (5,6) explicit Runge-Kutta pairs.

R.D. Skeel: Canonical Integration Methods for Molecular Dynamics

Abstract

We report on experiments with simulated liquid argon. Also we present a radical alternative to current variable stepsize strategies, which can preserve the property of being canonical and which is applicable to a wide range of practical problems.

B.D. Sleeman: The Dynamics of Reversible Systems and Spatio-Temporal Complexity in Biology

Abstract

Modelling the rich variety of complex and even chaotic phenomena observed in developmental biology, chemical physics and physiology presents a fundamental challenge to applied mathematics.

This lecture explores the complexity of nature through a number of models drawn from population genetics and physiology. In so doing, it is shown how the dynamics of reversible systems may be developed and applied to biological modelling.

The understanding of spatio-temporal chaos is one of the great challenges of applied mathematics. In the context of biology we shall propose a systematic way of making progress in certain areas and in so doing make contact with a type of Arnold diffusion.

D.M Sloan: Pseudospectral Techniques for Singular Problems

Abstract

Pseudospectral methods will be presented for singular perturbation problems and for problems with coordinate singularities. The latter type of problem arises in situations which involve cylindrical or spherical geometries.

M.Sofroniou: Symplectic Integration Schemes for General Hamiltonians to any Order

Abstract

Symplectic integration algorithms preserve the structure of Hamilton's equations and all the Poincaré invariants. Due to the nature of problems in Hamiltonian dynamics, long time integrations (sometimes more than a million iterations) and high orders are required. We are primarily concerned with the asymptotic and qualitative features of the dynamics. Conventional numerical integration techniques, such as explicit Runge-Kutta methods and Multi-step methods, fail to represent the dynamics faithfully; standard techniques are dissipative (local trajectories bunch together) whereas Hamiltonian systems are conservative. It has been shown that Symplectic (implicit) Runge-Kutta schemes exist. The familiar Gauss-Legendre schemes satisfy the necessary constraints for symplecticity but high order schemes prove computationally inefficient because stages are coupled together. Methods with weaker coupling between the stages are being derived, but require more stages to achieve the same order of accuracy.

This work concerns extending the results of Channel and Scovel. By using tensor notation the derivation of this class of methods has been simplified and generalised

to any order. Because of the necessity for high derivatives complicated algorithms may ensue. A symbolic package has therefore been written to derive the scheme for any specified Hamiltonian to any desired order. The resulting equations are implicit for position but, when these have been solved, the equations for momentum are explicit.

An Adams Bashforth predictor is used to obtain a good initial estimate for solving the implicit equations. The implicit equations are then solved using a Newton iteration scheme. This process has proved far more computationally efficient and robust than was previously considered possible.

A. Spence (with K.A. Cliffe and T.I. Garratt): The Numerical Detection of Hopf Bifurcations in Large Systems Arising in Fluid Mechanics

Abstract

Mixed finite element discretizations of equations modelling viscous incompressible flow produce nonlinear finite dimensional systems of the form

$$M\frac{dx}{dt} + H(x,\lambda)x + Lx + Cy = b, \; C^T x = c, \qquad (1)$$

where $\lambda \in R, x \in R^n, y \in R^m$, with $n > m$. Here M and L are symmetric positive definite $n \times n$ matrices, C is a $n \times m$ matrix of rank m, and $H(x,\lambda)$ is an $n \times n$ (generally nonsymmetric) matrix. For the two dimensional Navier-Stokes equations, the discretization we use has $n \approx 2m$ and $n+m$ is "large".

In many applications it is important to determine whether or not a steady state solution of (1), (x_0, y_0, λ_0) say, is *stable* with respect to small perturbations. After linearisation about the steady state the principle of linearised stability requires that we determine if there are any eigenvalues in the left half-plane of the generalised eigenvalue problem

$$Aw = \mu Bw \qquad (2)$$

where A and B are $(n+m) \times (n+m)$ matrices with the special block structure

$$A = \begin{bmatrix} K & C \\ C^T & 0 \end{bmatrix}, B = \begin{bmatrix} M & 0 \\ 0 & 0 \end{bmatrix},$$

and with $K = H(x_0,\lambda_0) + H_x(x_0,\lambda_0)x_0 + L$. Here K is nonsymmetric and B is (obviously) singular, and so standard software will be at best inefficient and probably not even feasible on large problems.

In this talk we discuss in detail the problem of the determination of the stability of steady state solutions of (1). A new method is described for the calculation of the eigenvalues of (2) of smallest real part, and these in turn answer the stability question. Numerical results are presented for three problems (a) double diffusive convection, (b) the Taylor problem, and (c) flow over a backward-facing step. The last problem involves the calculation of eigenvalues of (2) where $n + m \approx 2 \times 10^5$.
(*This work was supported by SERC.*)

A. Spence: see also F. Bai (with A. Spence & A.M. Stuart) and A. Champneys (with A. Spence and J. Toland)

M. Spijker: On Numerical Ranges and Stability Estimates

Abstract

In my lecture "On numerical ranges and stability estimates" I might touch upon the following subjects:

I The classical numerical range of a matrix, and the generalization known, in functional analysis, under the name "algebra numerical range".

II A generalization of the "algebra numerical range" published in Lin. Alg. Appl. (1990), under the name M-numerical range (Lenferink et al.).

III Relating the M-numerical range to

a) ϵ-pseudo-eigenvalues (Trefethen et al. 1990)

b) stability analysis of numerical methods for solving initial-value problems in ordinary and partial differential equations.

IV Basic properties of the M-numerical range

V Recent results and open problems related to stability estimates based on the use of M-numerical ranges.

D. Stoffer (with K. Nipp): Geometric Properties and Global Error Estimates for Stiff ODE Solvers

Abstract

Singularly perturbed systems of ODE's are a model class for so-called stiff systems which are difficult to treat numerically. Hairer et al. [1] (see also [2]) have studied the behaviour of implicit Runge-Kutta methods applied to singularly perturbed ODE's. They were able to prove that for those RK-methods the error of the method does not increase as the stiffness of the system increases.

Under the usual assumptions a singularly perturbed system has important geometric properties. More precisely, there exists an invariant manifold of the system which is smooth and highly attractive (cf. [4]). On the other hand, a numerical method applied to a system of ODE's defines a mapping in phase-space. In [3] it was shown that the map generated by the backward Euler method in fact has the same geometric properties as the underlying singularly perturbed ODE.

Here we prove an analogous result for stiff implicit RK-methods. We show that these methods not only perform well when applied to this model class but also preserve the important geometric property of the ODE. Moreover, the existence of the attractive invariant manifold leads to direct estimates of the global error.

[1] E. Hairer, Ch. Lubich, M. Roche *Error of Runge-Kutta methods for stiff problems studied via differential algebraic equations*, BIT, 28 (1988), 678-700.

[2] E. Hairer, G. Wanner, *Solving Ordinary Differential Equations II, Stiff and Differential-Algebraic Problems*, Springer, 1991.

[3] U. Kirchgraber, K. Nipp, *Geometric properties of RK-methods applied to stiff ODE's of singular perturbation type*, Research Report No. 89-02, Applied Mathematics, ETH Zurich, (1988).

[4] K. Nipp, *Invariant manifolds of singularly perturbed ordinary differential equations*, ZAMP, 36 (1985), 309-320.

R.F. Streater: The Free-Energy Theorem

Abstract

The theorem that free energy decreases along an orbit in an isothermal chemical system is deduced from Boltzmann's H-theorem by modelling the heat-bath as a system of heat particles which engage in reactions with the chemicals.

A. Stuart: The Dynamics of Local Error Control Mechanisms for Dissipative and Related Dynamical Systems

Abstract

The dynamics of numerical methods with local error control are studied for systems of ordinary differential equations. Two classes of equations are studied: *dissipative systems* where there is a bounded set which all trajectories eventually enter and remain in and *gradient systems* where the ω-limit point of an individual trajectory is contained within the set of equilibria.

Both error per step and error per unit step strategies are studied. Conditions on the tolerance for the error control are determined under which appropriate discrete analogues of the properties of the underlying differential equation may be proved.

A. Stuart: see also F. Bai (with A. Spence and A.M. Stuart) and C.M. Elliott (with A. Stuart)

E. Süli: The Analysis of Lagrange-Galerkin Methods for Evolutionary Problems

Abstract

The numerical modelling of convection and convection-dominated diffusion processes arises in various fields such as meteorology, oil reservoir simulation, magnetohydrodynamics, aerodynamics and geophysics. Unfortunately, when applied to problems of this type, most standard schemes suffer from stability-related time step limitations.

In recent years many numerical methods have been introduced which exploit the nearly hyperbolic nature of convection-dominated diffusion equations to overcome this difficulty. Lagrange-Galerkin methods are based on combining a time discretisation of the Lagrangian material derivative along particle trajectories with a spatial Galerkin projection. These methods are genuinely multi-dimensional and possess remarkable stability properties. In addition, they allow the use of large time steps at no cost in accuracy.

We present an analysis of Lagrange-Galerkin methods for convection-dominated diffusion equations. Both finite element and spectral Galerkin discretisations are considered. For the incompressible Navier-Stokes equations in two and three dimensions the Lagrange-Galerkin method is shown to be unconditionally nonlinearly stable and optimally accurate.

The theoretical results and the potentials of these schemes are illustrated by numerical experiments.

P.K. Sweby (with H.C. Yee): On Spurious Asymptotic Numerical Solutions of 2×2 Systems of ODEs

Abstract

The phenomenon that the asymptotic behaviour of a nonlinear differential equation and its discretized counterpart can have different dynamical behaviour was not uncovered fully until recently. In earlier work we discussed some of the differences between the dynamics of scalar first-order autonomous nonlinear ODEs and commonly used ODE solvers. In this presentation we investigate numerically the dynamical behaviour of numerical discretizations of 2×2 systems of first-order autonomous nonlinear ODEs. Our goal is to illustrate the interplay between the occurrence of spurious fixed points, limit cycles and numerical basins of attraction, and the phenomenon of incorrect, non-convergent and divergent numerical solutions of a class of Runge-Kutta methods.

Q. Tang: Contact Problems in Dynamical Thermoelasticity

Abstract

An evolutionary problem arising in linear thermoelasticity is considered. Using methods of penalization and compensated compactness, an existence result is obtained for the wave equation coupled with the heat equation together with a unilateral boundary condition of Signorini type.

Tao Tang:
The Hermite Spectral Method and Scaling Factor

Abstract

Although Hermite functions were widely used for many practical problems, numerical experiments with the standard (normalized) Hermite functions $\psi_n(v)$ worked poorly in the sense that too many Hermite functions are required to solve differential equations. In order to obtain accurate numerical solutions it is necessary to choose a scaling factor α and use $\psi_n(\alpha v)$ as the basis functions. In this paper the scaling factors are given for functions which are of Gaussian type, which have finite supports $[-M, M]$. The scaling factor we used is $\max_{0\leq j\leq N}\{\gamma_j\}/M$, where $\{\gamma_j\}_{j=0}^N$ are the roots of $\psi_{N+1}(v)$ and $N+1$ is the number of the truncated terms used. The numerical results show that after using this scaling factor only reasonable numbers of the Hermite functions are required to solve differential equations.

J. Terjéki:
Stability and Asymptotic Stability for Pantograph Equations

Abstract

The equation

$$y'(t) = a(t)y(t) + b(t)y(pt) + c(t)y'(qt) \quad (1)$$

and its nonlinear generalization

$$y'(t) = f(t, y(t)) + g(t, y(pt)) + c(t)y'(qt) \quad (2)$$

are considered, where

$$a, b, c : [0, \infty) \longrightarrow C,$$

$$f, g : [0, \infty) \times (-\infty, \infty) \longrightarrow C$$

are bounded functions,

$$\sup_{t\geq 0} | c(t) | \leq 1$$

and p, q are real constants with $0 < p, q < 1$. Conditions are given for the asymptotic stability of the zero solution via Liapunov - like functions and the validity of the estimate

$$| y(t) | \leq \frac{c_1 | y_0 |}{(1 + c_2 t^{c_3})^{c_4}}$$

is shown, with some positive constants c_i.

L. Torelli and R. Vermiglio (with V.B. Kolmanovskii):
Stability of Some Test Equations with Delay (Parts 1 & 2)

Abstract

The authors propose the use of degenerate Liapunov functionals to derive sufficient conditions for stability of certain differential equations with delay. There is also a numerical interest in this investigation: for the analysis of the stability properties of the numerical approximation schemes it is important to have a set of general test equations.

In the first part the authors consider the following scalar real equation

$$x'(t) = -\sum_{i=1}^{N} b_i(t)x(t - \tau_i(t)), \quad t \geq 0$$

with the initial condition $x(t) = \phi(t)$ for $t \leq 0$, without an instantaneous dissipative term. This model is important for practical purposes, for instance in control theory, where the instantaneous feedback is not realizable.

In the second part they consider the scalar real equation

$$x'(t) = a(t)x(t) - \sum_{i=1}^{N} b_i(t) \int_0^\infty x(t - s)dk_i(s), \quad t \geq 0$$

with the initial condition $x(t) = \phi(t)$ for $t \leq 0$, where $k_i(t)$ are functions in $[0, \infty)$ with bounded variation. It is important to point out that sufficient conditions for asymptotic stability of this test equation do not imply that the coefficient $a(t)$ must be negative.

K. Wright:
Numerical Solution of ADEs for the Analytic Singular Value Decomposition of a Matrix

Abstract

It is well known that any $m \times m$ matrix has a singular value decomposition (SVD) and that there is some freedom of choice in this decomposition. For matrices depending smoothly on a parameter t there exists an SVD for each parameter value, but it is not immediately clear whether it is possible to choose within the available freedom, a decomposition which is similarly smooth. To avoid pathological cases it is convenient to restrict consideration to the case where the elements of all the matrices are analytic functions of the parameter.

It is shown that the factors of the SVD satisfy a system of differential algebraic equations. These equations provide an alternative approach to the discussion of existence and further insight into the freedom of choice for the ASVD.

They also form the basis for alternative numerical methods. The solution of these equations is reasonably straightforward except at points where there are singular values equal in modulus. A modified explicit Runge Kutta solver was developed to deal with these exceptional points. This often works well but there are difficulties in choosing suitable tolerances and also using automatic step adjustment very small step sizes are sometimes taken near these exceptional points making the method expensive.

An alternative approach is to use collocation-implicit Runge Kutta based on Gauss points. Full (Newton) linearization of these non-linear equations is expensive, but often gives good results. Simple iteration fails near the exceptional points. An alternative partial linearization method is suggested.

A sub-problem is the solution of a differential system with an anti symmetric coefficent matrix. Equations of this type preserve scalar products for different solutions. A result related to B-stability theory shows that numerical solution using Gauss point collocation also preserves such scalar products.

Results will be presented illustrating the different methods.

M. Zennaro:
Waveform Relaxation Iterative Schemes based on Runge-Kutta Methods

Abstract

We consider a very general class of waveform relaxation iterative schemes, which are based on Runge-Kutta methods, for the numerical solution of initial value problems for large systems of ordinary differential equations.

We discuss briefly the potential of such schemes for implementation in a parallel computing environment. Then we give general results about their convergence properties on arbitrarily long windows and about their order of accuracy.

M. Zennaro: see also Z.Jackiewicz (with A. Bellen and M. Zennaro)

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