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DISCLAIMER

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Tuesday AM

PLENARY SESSION

A DAE Black-box Solver Complete with Owner's Manual: What's there, What's needed

S.L. Campbell

Computer simulation of ordinary differential equations is widely used in every discipline in science and engineering. The complexity of the models considered is steadily increasing as is the use of simulation during the initial phase of design and experimentation when the model may be frequently altered. Many of these systems are most easily initially formulated as differential algebraic equations (DAEs). An ultimate goal would be to have a Black-box DAE solver that would enable, say a biologist, or a mechanical engineer, to write down a bunch of equations and relations, drop them into the box, and watch the simulation take place. This talk will examine how close at least a "Grey-box" is.

Some of the problems special to DAEs will be discussed and existing DAE codes and methods surveyed. Then we will discuss what kinds of algorithms are needed for the "decision making" part of the blackbox. Needed numerical theory and algorithms will be discussed. Throughout the talk our emphasis will be on making the box as black as possible. That is, reducing the amount of DAE and ODE integrator knowledge required of a potential user.

Error Growth in the Numerical Integration of Periodic Orbits

J.M. Sanz-Serna

We analyse the growth with time of the error in the numerical integration with one-step methods of periodic solutions of systems of ordinary differential equations. We consider 'general', Hamiltonian and reversible systems. For Hamiltonian and reversible systems, numerical methods with relevant geometric properties are proved to have better error growth than 'general' methods.

PARALLEL A: ODE SOFTWARE

CVODE, A Stiff/Nonstiff ODE Solver in C

S. Cohen and A. Hindmarsh

CVODE is a package written in ANSI standard C for solving initial value problems for ordinary differential equations. It solves both stiff and nonstiff systems. In the stiff case, it includes a variety of options for treating the Jacobian of the system, including dense and band matrix solvers, and a preconditioned Krylov (iterative) solver. CVODE provides the capabilities of two older Fortran packages, VODE and VODPK, written by Brown, Byrne, and Hindmarsh.

The integration methods in CVODE are Adams and BDF methods, at user option. Corrector iteration is by functional iteration or Newton iteration. For the solution of linear systems within Newton iteration, users can select a dense solver, a band solver, a diagonal approximation, or a preconditioned Generalized Minimal Residual (GMRES) solver. In the dense and band cases, the user can supply a Jacobian approximation or let CVODE generate it internally. In the GMRES case, the preconditioner is user-supplied.

CVODE is organized in a highly modular manner. The basic integrator module is separate from, and independent of, the linear system solvers. Thus the set of linear solvers can be expanded in the future, with no impact on the integrator. All operations on N-vectors (where N is the system size) are isolated in a set of vector kernels. Except in the diagonal approximation case, each linear solver module called by CVODE in turn makes calls to a generic solver based on a dense, banded, or preconditioned GMRES method.

In addition to the goal of producing an ODE solver in C, the design and development of CVODE was done with a second purpose in mind. From CVODE, we plan to produce a family of extensions, called PVODE, for massively parallel machines. PVODE will adopt the SPMD (Single Program, Multiple Data) programming model. Initial versions of it will be accomplished primarily by substituting parallel versions of the vector kernels for those in CVODE.

The choice of C as the language for CVODE was motivated in large part by the planned parallel extension, and also by numerous flexibility features not available in Fortran. CVODE makes extensive use of dynamic memory allocation, pointers, and structures. We prefer C over C++ because of C's wider availability and uniformity, and the greater ease of interfacing C with applications written in extended Fortran. CVODE accommodates single and double precision with a single source by way of a header file containing type definitions.

CVODE has been made available in Netlib, and the package includes an extensive user guide.

An Object-Oriented Approach to ODE Codes

A. Hohmann

This talk presents some of our experiences using object-oriented techniques for the implementation of ODE codes. These techniques may be applied to the two sides of an ODE solver: the interface describing the given ODE problem, and the implementation of the solver itself. In fact, both questions are strongly related, since one integration method may use more or different information about the ODE than another.

Concerning the description of the ODE, the main objective is an easy-to-use interface which nethertheless allows us to exploit the particular structure of the ODE. As an example, we may wish to use a suitable sparse or iterative solver for the linear equations arising in implicit discretization schemes. One may also think of different scaling strategies adopted to the particular problem.

Our approach to adaptive integration codes is strongly influenced by the fact that many codes use similar mechanisms to control the stepsize during the integration process. The starting point for our investigation is the well-known set of extrapolation codes EULEX, EULSIM, DIFEX, etc., by Deuflhard and his co-workers. All of these codes are based on the same order and stepsize control, combined with extrapolation, but use different discretization schemes such as the explicit or linearly implicit euler scheme, or the explicit mid-point rule. Thus, it is natural to encapsulate the common structures and to use them for the different integration methods, thus separating the stepsize control from the discretization schemes.

We propose a set of objects (realized as C++ classes) which have been successfully used for a large variety of ODE problems including different discretizations of time-dependent PDEs. In particular, these structures are not confined to extrapolation codes, but may be used for other integration methods, too. We also address crucial questions such as storing information during the integration process (e.g., for continuous output), as well as the performance of the resulting codes in comparison to procedural implementations.

TERK: A New Explicit Continuous Runge-Kutta Package

W. H. Enright

Almost twenty years ago we implemented, in the DVERK package [2], an explicit discrete Runge-Kutta formula pair derived by Verner. The user options associated with the package and the user interface were at the state-of-the-art for that time period. Since then new improved formulas have been proposed, continuous extensions of discrete methods have been developed, and various heuristic strategies (associated with an implementation) have been improved.

In addition to these advances in the analysis and development of Runge-Kutta methods there has been a dramatic change in the background of the user community that such software packages are serving. Increasingly these packages are being used as 'black boxes' in high-level problem solving environments by non-technical users who are not aware of the limitations and inherent difficulties that can arise in the numerical solution of initial value problems. For such users it is very important that the packages that are adopted be reliable and robust and that the solutions produced

(associated with different options) be as consistent as possible even if this requires some sacrifice in efficiency.

For the last six years we have been involved, at the University of Toronto, in developing an explicit continuous Runge-Kutta software package, TERK, that adopts some of the advances made in the analysis of numerical methods and also addresses the demands of the changing user community. In this talk we will discuss the evolution of this project and the key features of TERK that distinguish it from DVERK and from the recently developed package RKSUITE [1].

References

[1] R. W. Brankin, I. Gladwell, and L. F. Shampine, *RKSUITE: A suite of explicit Runge-Kutta codes*, in Contributions in Numerical Mathematics, R. Agarwal, ed., World Scientific, Series in Applicable Analysis, vol II, 1993, pp. 41-53.

[2] T. E. Hull, W. H. Enright, and K. R. Jackson, *User's guide for DVERK—a subroutine for solving non-stiff ODEs*, Tech. Report 100, University of Toronto, 1976.

RKLAG/DRAKE: Codes for the Solution of Ordinary and Delay Differential Equations

S.C. Corwin and S. Thompson

We describe the features and illustrate the usage of the RKLAG and DRAKE codes. RKLAG is a suite of subroutines designed to solve nonstiff systems of delay differential equations with state dependent delays. It also may be used to solve systems of ordinary differential equations which do not contain delays. DRAKE is an interactive PC interface which simplifies the usage of RKLAG.

RKLAG is based on a pair of continuously imbedded Runge–Kutta–Sarafyan methods. It incorporates several noteworthy features including heuristics similar to those used in well–known Runge–Kutta codes for ordinary differential equations, interpolation to handle dense output, root finding involving the solution, automatic location of points of derivative discontinuities, nonstandard interpolation of the solution history queue, provision to solve vanishing delay problems, and detailed error diagnostics. It is written in f77 FORTRAN and conforms to the programming conventions of the SLATEC mathematical software library (*e.g.*, machine dependencies and diagnostic output are localized in a few relevant subroutines and functions).

Usage of RKLAG may be simplified through the use of the interactive menu–driven PC interface DRAKE which prompts the user for necessary problem information and writes the necessary subroutines and main program (which may then be used on a PC or ported to any machine with an f77 compiler) required by RKLAG. DRAKE provides a standard interface which sets default parameters and it contains an optional "expert menu" which allows the user to take advantage of the full range of RKLAG options. It also allows the user to conveniently obtain plots of the solution and auxiliary variables when used in conjunction with D. K. Kahaner's Volksgrapher graphics package (available via anonymous ftp from the National Institute of Standards). DRAKE is similar to well–known continuous simulation languages in these respects. Consequently, it also may be used also for teaching purposes in elementary differential equations courses in which students have limited a

knowledge of FORTRAN as well as in advanced courses which include complex models with delays.

Examples will be given to illustrate the available features and usage of both codes. Single and double precision versions of RKLAG and the DRAKE interface are available along with supporting documentation and test programs via anonymous ftp. Email correspondence and inquiries regarding RKLAG and DRAKE should be addressed to thompson@reed.science.runet.edu.

PARALLEL B: PARAMETER ESTIMATION AND DESIGN OPTIMIZATION

Many differential equation models contain parameters whose values are chosen to optimize performance in some way while satisfying certain constraints. Design optimization and parameter estimation problems typically contain only a few discrete parameters, while optimal control problems often contain infinite dimensional parameters that may vary in space and time. Finite-dimensional optimization algorithms can be applied to discretizations of these problems, but some important issues arise. Discretization techniques and algorithms must respect the infinite-dimensional nature of the underlying continuous problem; and the structure of the discrete problem must be exploited to make the method efficient.

The talks in this session describe algorithms for parameter estimation and control problems. Aspects to be discussed include stability and efficiency of algorithms, applications to engineering problems, and parallel implementation.

Optimization Methods for Large Scale Constrained Control Problems

M. Heinkenschloss

This talk is concerned with the efficient numerical solution of optimal control problems with control constraints that are governed by nonlinear partial differential equations. Such problems lead to very large constrained optimization problems with an infinite dimensional structure.

We investigate methods that combine sequential quadratic programming (SQP) methods, interior point methods, trust region strategies, and multilevel preconditioned Krylov subspace methods. These methods treat states and controls as independent variables and, as a consequence, only require the solution of the linearized state equation. The interior point and trust region approaches preserve the structure of the unconstrained control problem and allow an efficient solution of the subproblems using preconditioned Krylov subspace methods. We discuss the theoretical properties of these optimization methods and their application to control problems governed by a nonlinear heat equation and the nonlinear Navier–Stokes equations.

Parallel BVP Algorithms for Parameter Estimation: Chemical and Mechanical Applications

J.P. Schloeder

Mathematical modelling of dynamical processes frequently leads to complex nonlinear systems of ordinary or differential algebraic equations. Typically some parameters in these systems have to be estimated from measurements to guarantee a sufficient agreement of model reponse with reality. The talk describes adequate mathematical formulations of these problems and points out typical properties and structures that are exploited by efficient numerical algorithms. Boundary value problem methods have proven to be very successful for the solution of this class of parameter estimation problems. The talk outlines how DAE models are discretized e.g. by multiple shooting or collocation and what kind of structures occur in the resulting constrained nonlinear optimization problems which are subsequently solved by tailored Gauss-Newton or SQP methods. It is shown where parallelism occurs and how it is exploited in the generation and solution of the quadratic subproblem. Since measurements may be costly or time-consuming, algorithms for the determination of optimum experiment strategies are sketched. Emphasis is laid on demonstrating the performance of the new parallel algorithms. Numerical results are given for parameter estimation problems in nonlinear, chaotic and stiff dynamical models in reaction kinetics, chemical engineering, mechanics and related fields. The computations are performed on PowerPC transputer systems.

The results reported were obtained in joint work with Hans Georg Bock and Johanna Gallitzendoerfer

Algorithms for Linear ODE Problems with Parameters and Side Conditions

S. Wright

Conditioning of two-point boundary value ODEs is well understood in terms of fundamental solution modes, according to a theory developed in the early 1980s. This theory has given valuable insight into the stability of algorithms. It was partially extended during the late 1980s to ODEs with parameters or side conditions.

In this talk we discuss an alternative view of comditioning based on the perturbation theory of numerical linear algebra developed in a book by o Stewart and Sun. This viewpoint allows us to quantify the conditioning of problems when both overdetermined side conditions and parameters are present. We also discuss efficient algorithms for solving the linear equations and linear least squares problems that arise after discretization. These methods include structured orthogonal factorization, partitioned compactification, and cyclic reduction. Often, the methods are easy to describe and analyze for two-point boundary value problems, but become more complex with the addition of side conditions and parameters. Parallelizability is a key feature of these methods. Finally, the stability theory is used to demonstrate stability of the algorithms. The theory also predicts how much extra work the algorithm needs to perform to circumvent degeneracy in the block-banded part of the coefficient matrix.

PARALLEL C: VALIDATED COMPUTATIONS

Introduction to Validated ODE Solving

G.F. Corliss

The purpose of this talk is to provide an introduction to interval techniques for the validated computation of solutions to initial value problems in ordinary differential equations (ODEs) $y' = f(t, y)$, $y(t_0) = y_0$. This talk will set the stage for the other talks in this minisymposium. We show from the Picard Iteration Theorem that validated enclosures are feasible. Computing guaranteed bounds for the range of f over a region containing (t_0, y_0) leads to an interval-valued function $[y](t)$ that encloses the true solution $y(t)$ in a neighborhood of t_0. There are several excellent surveys of interval techniques for ODEs including Bauch 1989, Corliss 1989, Corliss 1994, Nickel 1986, Rihm 1994, Stetter 1986, and Stetter 1990. Extensive bibliographies to literature in the field may be found in the survey papers and in Corliss 1988 or Corliss 1991.

The most widely used software for the validated solution of ODEs, is AWA (Anfangswertaufgabe) by Rudolf Lohner (1978, 1987, and following). Lohner attempts to minimize the wrapping effects by representing the enclosure of the solution at each time step as a linear transformation of an interval: $u(t_j) \in A_0 \cdots A_{j-1}[x_j]$ at time $t = t_j$. He advances the solution to $t = t_{j+1} := t_j + h$ using two algorithms:

Algorithm I. Validate existence and uniqueness using Picard-Lindelöf iteration

Input:
- Problem: $u' = f(t, u)$ — Final time: t_f
- Initial conditions: t_j, $u(t_j) \in [u_j]$ — Tolerance

Output:
- Coarse enclosure: $[u_j]_0$ — Step size: h

Output assertions:
- $u' = f(t, u)$, $u(t_j) = u_j \in [u_j]$ has a unique solution in $[t_j, t_j + h] \times [u_j]_0$
- $u(t) \in [u_j]_0$ for all $t \in [t_j, t_j + h]$

Algorithm II. Compute tighter enclosure using Taylor series and local coordinate transformation

Input:
- Results from Algorithm I

Output:
- Matrix: A_j
- Interval: $[x_{j+1}]$
- Next node: $t_{j+1} \leq t_j + h$
- Solution: $[u_{j+1}] :=$ Convex hull $(A_0 A_1 \cdots A_j [x_{j+1}])$ with $w([u_{j+1}])$ <= Tolerance

Output assertion:
- $u(t_{j+1}) \in A_0 A_1 \cdots A_j [x_{j+1}]$

We give a worked-out numerical example.

Step Size and Order Control in the Verified Solution of Ordinary Initial Value Problems

R. J. Lohner

In the past self-validating methods for the solution of ordinary initial value problems were usually designed and implemented with constant step sizes and fixed order. Also, most methods, being explicit, do not allow step sizes which are larger than an Euler step due to the so called a priori enclosure step which is used by these methods in order to guarantee the existence of the solution for the complete time step under consideration. However, since these methods are usually based on local Taylor-expansions there is no need for these restrictions. The drawback of small Euler steps can be overcome by a modified a priori enclosure step using interval polynomials of higher degree. Then step size and order can be controlled in a way analogously to classical approximation methods, however, in our self verifying context we take advantage of the knowlegde of safe bounds for the local and global discretization errors. now allows step sizes larger than an Euler step, by using a suitable interval polynomial arithmetic. Additionally, the method is supplemented by a step size control which basically is due to Eijgenraam (1981). These two extensions yield a much more powerful and flexible enclosure method for initial value problems than the previous method has been. The extensions will be presented, discussed and demonstrated with many numerical examples.

Discontinuous Right-Hand Sides

R. Rihm

We consider the problem

$$u' = f(t,u) = \begin{cases} f^-(t,u), & g(t,u) < 0 \\ f^+(t,u), & g(t,u) > 0 \end{cases},$$
$$u(t_0) = u_0 \in \mathrm{int}(D) \subseteq \mathbb{R}^n,\ t_0 = \inf(I),\ I \in \mathbb{IR},$$

($\mathbb{IR}$ is the set of all closed intervals in $\mathbb{R}$) where $f^-, f^+ : I \times D \to \mathbb{R}^n$, and $g : I \times D \to \mathbb{R}$ are continuously differentiable. The set $\{(t,u) \in I \times D | \, g(t,u) = 0\}$ is called the *switching space* of the ODE system. A continuous function $u^*(t)$ is called a solution of the initial value problem if it satisfies $u^*(t_0) = u_0$ and $u^{*\prime}(t) = f(t,u^*(t))$ almost everywhere in its domain. If certain *transversality conditions* are fulfilled, the graph of the solution crosses the switching space at the *switching points*, where it is not differentiable in general.

We can enclose the solution outside the switching space using a method for the "continuous case" (eg. Lohner's method). At the switching points, the right-hand side of the differential equation changes. The enclosure method has to be restarted. Unfortunately, the switching points are not known *a priori* and they cannot be computed exactly. In the talk, we discuss several strategies to overcome these difficulties. The main tools are a Newton-like iteration algorithm to enclose the switching points and a particular two-step method to enclose the solution while crossing the

switching space. The algorithms can be combined with Lohner's method or any other enclosure method for initial value problems. Numerical results demonstrate their effectiveness.

A Numerical Method for the Validation of Solutions of Differential-Algebraic Equations

W. A. Lodwick and A. Neumaier

We discuss a semilocal existence theorem for solutions of singularly perturbed or differential-algebraic initial value problems of the form $Ay' = f(x, y)$ with a singular (or very ill-conditioned) matrix A. The hypothesis of the theorem can be verified constructively on a computer, provided that a sufficiently accurate approximation to the solution is available, and the problem is nondegenerate (index at most one). The existence theorem can therefore be used to verify the accuracy of such approximations. For singularly perturbed or differential-algebraic boundary value problems, the validation of a solution can be achieved by combining the above existence theorem with a multiple shooting method with adaptive spacing and a sparse linear interval equation solver.

PARALLEL D: SINC METHODS

Overview of Sinc Methods for ODE and PDE

F. Stenger, J.Lund and K. Bowers

Sinc Methods for Initial Value Problems

T. Carlson

Sinc–Collocation for Elliptic Problems

N. Lybeck

Sinc Domain Decomposition Methods

A. Morlet

Tuesday PM

PLENARY SESSION

Preserving Positivity and Monotonicity in the Numerical Solution of Riccati Equations

*L. Dieci**

In this talk, we consider differential Riccati equations of the type arising in optimal control problems, that is, Riccati equations associated to (dichotomic) linear Hamiltonian systems. Solutions of these equations satisfy two key properties: (i) they are positive (semi)definite matrices if the initial conditions are, and (ii) they are monotone –with respect to the ordering of positive matrices– if the data are. These properties are crucial for both theoretical and practical reasons.

We will discuss when these properties are maintained under discretization. As it turns out, no direct discretization can generally maintain positivity (or monotonicity) and have order greater than one. However, indirect solution procedures are possible, whereby one recovers the solution of the Riccati equation via the solution of some associated problem. In this case, there exist schemes leading to arbitrarily high order approximations for the Riccati equation. In particular, Gauss-Runge-Kutta schemes on the underlying Hamiltonian system eventually recover positivity and monotonicity in the solution of Riccati equations.

* Joint work with Timo Eirola, Dept. of Mathematics, Helsinki University of Technology.

Computations of Travelling Waves and Connecting Orbits

W. Beyn

Travelling waves in PDE's can be computed by solving a boundary value problem for an ODE on the real line. In the phase space of this ODE the corresponding orbit connects two steady states. Such connecting orbits are of independent interest because they also arise in global bifurcations of dynamical systems.

In this talk I will discuss the following questions. How do the error estimates look like when instead of the infinite b.v.p. we solve numerically a finite b.v.p. with asymptotic boundary conditions ? Does this generalize to orbits which correspond to more complex solitary waves, e.g. those which connect a steady state to a periodic orbit ? How does the spectrum of the linearized finite b.v.p. relate to the stability of the wave ?

PARALLEL A: LONG–TIME INTEGRATION

Asymptotic Stability of One–Leg Methods for Dissipative Differential Equations

A. T. Hill

Dissipative evolutionary ODEs and PDEs are characterized by the existence of a bounded set, which all trajectories eventually enter and remain inside. This talk summarises recent work giving necessary and sufficient conditions for one–leg multistep time discretizations of such problems to preserve this dissipative behaviour.

The underlying theory, which extends Dahlquist's work on G–stability, relies on the identification of a family of norms in which the numerical solution is actually strictly contractive in the complement of a bounded subset of phase space, rather than merely stable — i.e. non–expansive.

These techniques have been applied to show the existence of a global attractor for a second–order accurate discretization of the incompressible Navier–Stokes equations, using finite–elements in space and a semi–implicit version of the second BDF method in time.

Structural Stability of ODE's with respect to Discretization

B. M. Garay

Generalizing and unifying the corresponding results of Beyn, Eirola, Fečkan, Kloeden, J. Lorenz and others, discretization analogues of several well-known theorems from the qualitative theory of ordinary differential equations are presented.

One-step discretization methods of the form $\varphi : [0, h_0] \times \mathbf{R}^n \to \mathbf{R}^n$ are considered. It is assumed that φ is $(p+1)$-times (p is a positive integer) continuously differentiable, with all derivatives bounded and that
$|\varphi(h,x) - \Phi(h,x)| \leq \text{const} \cdot h^{p+1}$, $(h,x) \in [0,h_0] \times \mathbf{R}^n$ where Φ is the solution flow of the autonomous equation $\dot{x} = f(x)$, $x \in \mathbf{R}^n$. It is also assumed that function $f : \mathbf{R}^n \to \mathbf{R}^n$ is $(p+1)$-times continuously differentiable, with all derivatives bounded. The basic result is that, for stepsize sufficiently small, transversal and hyperbolic structures are correctly reproduced by discretization. Moreover, in many cases, discretization is equivalent to the introduction of a new coordinate system.

The following qualitative concepts are investigated: a.) saddle-point structures about hyperbolic equilibria [1], [4] b.) normally hyperbolic invariant manifolds [3] c.) structural stability [2], [5], [6] d.) estimates in various topologies [7] e.) embeddability of the discretized system into a flow [8].

THEOREM [3]: Let φ, Φ, f as above and let $M \subset \mathbf{R}^n$ be a C^{p+1} compact normally hyperbolic invariant manifold for $\dot{x} = f(x)$. Then, for all h sufficiently small, there exists a C^p embedding $F_h : M \to \mathbf{R}^n$ such that $M_h = F_h(M)$ is a normally hyperbolic invariant manifold for $\varphi(h,\cdot) : \mathbf{R}^n \to \mathbf{R}^n$. Further, with d_j denoting the norm distance in $C^j(M, \mathbf{R}^n)$, there holds
$d_j\ (F_h, \text{inclusion}_M) \leq \text{const} \cdot h^{p-j}$, $j = 0, 1, \ldots, p$.

THEOREM [5]: Let $\mathcal{D}^n$ be the unit disc in $\mathbf{R}^n$ and assume that $p \geq 3$. Further, assume that f defines a Morse-Smale system without periodic orbits on $\mathcal{D}^n$ and points inward on $\partial\mathcal{D}^n$. Then, for all h sufficiently small, there exists a homeomorphism $\mathcal{H}_h : \mathcal{D}^n \to \mathcal{H}_h(\mathcal{D}^n) \subset \mathbf{R}^n$ such that $\mathcal{H}_h(\Phi(h,x)) = \varphi(h, \mathcal{H}_h(x))$ and $|\mathcal{H}_h(x) - x| \leq \text{const} \cdot h^p$ whenever $x \in \mathcal{D}^n$.

[1] *Discretization and some qualitative properties of ordinary differential equations about equilibria*, Acta Math. Univ. Comenianae **62** (1993), 249–275.

[2] *Discretization and Morse-Smale dynamical systems on planar discs*, Acta Math. Univ. Comenianae **63** (1994), 25–38.

[3] *Discretization and normal hyperbolicity*, Z. angew. Math. Mech. **74** (1994), T662–T663.

[4] (with B. Aulbach) *Discretization of semilinear differential equations with an exponential dichotomy*, Computers Math. Applic. **28** (1994), 23–35.

[5] *On structural stability of ordinary differential equations with respect to numerical methods*, Numer Math., submitted

[6] *The discretized flow on domains of attraction: a structural stability result*, Fund. Math., submitted

[7] *On C^j-closeness between the solution flow and its numerical approximations*, J. Difference Eq. Appl., submitted

[8] *On various closeness concepts in numerical ODE's*, Computers Math. Applic., submitted.

Geometric Properties of Stiff Integration Schemes

K. Nipp

It is shown that appropriate linear multi-step methods (LMMs) applied to singularly perturbed systems of ODEs preserve the geometric properties of the underlying ODE. If the ODE admits an attractive invariant manifold so does the LMM. The continuous as well as the discrete dynamical system restricted to their invariant manifolds are no longer stiff and the dynamics of the full systems are essentially described by the dynamics of the systems reduced to the manifolds. These results may be used to transfer properties of the reduced system to the full system. As an example the global error of LMM-approximations to singularly perturbed ODEs is derived.

Long Time Integration with Reversible, Variable Steps

D. Stoffer

Conventional variable-step implementation of symplectic or reversible integra tion methods distroy the symplectic or the reversible structure of the system. I n order to preserve the symplectic structure of a method the step-size has to be kept almost constant. For reversible methods variable steps are possible, howev er, but the step-size has to be equal for "reflected" steps. We demonstrate po ssible ways to construct reversible variable step-size methods. Numerical experi ments show

that for the Kepler problem the new methods perform better than conve ntional variable step-size methods or symplectic constant step-size methods. In particular they exhibit linear growth of the global error (as symplectic methods with constant step-size).

PARALLEL B: DELAY DIFFERENTIAL EQUATIONS

Dynamics of Discretized Equations for DDEs

C.T.H. Baker

The classical LMF and RK formulae for ordinary differential equations [ODEs], can be extended to discretize DDEs

$$u'(t) = F(u(t), u(t-\tau)) \quad (t \geq 0) \quad u(t) = \psi(t) \quad t \in [-\tau, 0].$$

In this note, we establish that discretized delay differential equations [discretized DDEs] can display irregular dynamical behaviour similar to that seen in discretized evolutionary problems in ODEs of the form

$$y'(t) = f(y(t)), \quad (t \geq 0) \quad y(0) = y_0.$$

(The substitution $f(y) := F(y, y)$ is instructive if one seeks a general theorem.) In particular, the following phenomena can occur with simple linear multistep and Runge-Kutta formulae:

(i) spurious steady states using fixed stepsizes and adaptive stepsize strategies;

(ii) missing steady states using fixed stepsizes and adaptive stepsize strategies.

For the DDEs there is *greater* scope for irregular behaviour, in addition to that found for ODEs. Thus, one has the possibility of spurious cycles (using fixed stepsize strategies) depending on the ratio of the lag τ to the stepsize h.

Such phenomena are associated with nonlinear problems, and for implicit methods the question of solvability of the nonlinear equations enters the discussion. We shall use simple formulae to illustrate the analysis.

Stability of Discrete Volterra Equations

V.B. Kolmanovskii

The talk will be devoted to stability of equilibrium for Volterra equations with discrete time. Firstly, general stability theorems formulated in terms of auxiliary Liapunov functions will be proved. But the main part of the talk is to propose formal procedure (algorithm) to construct Liapunov functions for discrete Volterra equations in explicit form. It allows us to obtain stability conditions immediately in terms of the coefficients for different types of Volterra discrete time equations. Various illustrative examples and comparison with stability results obtained by another methods will be given.

Efficient Evaluation of Generalized Hypergeometric Functions via Functional Differential Equations

Y. Liu

It is found in a recent work by A. Iserles and I that generalized hypergeometric functions (GHFs) are solutions of some functional differential equations. Therefore, we can evaluate GHFs by solving these equations numerically. One obvious reason for this approach is that GHFs, if expressed as series, are difficult to evaluate for large argument. In this paper, we develop efficient numerical methods for solving these equation.

The Stability of Runge–Kutta Methods for Systems of Delay Differential Equations

K. in 't Hout

We consider Runge–Kutta methods for the numerical solution of initial value problems for systems of delay differential equations,

$$(*) \qquad U'(t) = f(t, U(t), U(t-\tau)) \quad (t \geq 0), \quad U(t) = g(t) \quad (t \leq 0),$$

where $\tau > 0$ denotes a given, constant delay. The adaptation of Runge–Kutta methods to $(*)$ is obtained by applying the general interpolation procedure from [1].

In our talk, we investigate the stability of the numerical methods under consideration. We assess the stability of the numerical methods by analyzing their behaviour in the case of

$$(**) \qquad U'(t) = LU(t) + MU(t-\tau) \quad (t \geq 0), \quad U(t) = g(t) \quad (t \leq 0),$$

where L, M are constant, square matrices. Our results generalize the results of [2], where the family of θ–methods was considered, and of [3], where a sufficient condition for stability in the case of $(**)$ was derived.

- [1] K.J. in 't Hout (1992): *A new interpolation procedure for adapting Runge–Kutta methods to delay differential equations.* BIT **32**, 634–649.
- [2] K.J. in 't Hout (1994): *The stability of θ–methods for systems of delay differential equations.* Ann. of Numer. Math. **1**, 323–334.
- [3] T. Koto (1994): *A stability property of A–stable natural Runge–Kutta methods for systems of delay differential equations.* BIT **34**, 262–267.

Equilibrium States, ODEs with Delay and Local Error Control

D. Higham

Standard software for evolutionary problems uses a *local* measure of error to adapt the timestep. Does this help in computing *long time* solutions? Two questions that have been investigated for ODEs are

- Does the algorithm avoid spurious fixed points?
- Does the algorithm behave well around true fixed points?

We will discuss how results in this area might be carried over to functional ODEs, especially those with logistic-type reaction terms.

Stability Analysis of Numerical Methods for Delay Differential Equations

M. Zennaro

We present a brief survey of the various test problems adopted in the literature for analyzing stability properties of numerical methods for delay differential equations DDEs) of the form $y'(t) = f(t, y(t), y(t-\tau))$. We consider mostly extensions of the classical test problems for ordinary differential equations (ODEs), namely $y'(t) = ay(t) + by(t-\tau)$ and $y'(t) = a(t)y(t) + b(t)y(t-\tau)$, up to the most general system of nonlinear equations. Then we present some of the most important results which have been found for the class of Runge-Kutta methods.

PARALLEL C: RECENT ADVANCES IN NUMERICAL TWO–POINT BOUNDARY VALUE PROBLEMS

There has been an extensive amount of research on numerical methods for two-point boundary value problems. This minisymposium will examine various new directions in this area and the progress that has been made in solving these kinds of problems. G. Bock will present boundary value algorithms for optimization and optimal control. J. Cash will discuss continuation methods for stiff boundary value problems. P. Lin will describe the sequential regularization method for boundary value DAEs. E. van Vleck will consider the theory and implementation of contimuous orthonormalization methods.

Parallel Optimization Algorithms for Boundary Value Problems for Higher Index DAE

H.G. Bock

Higher index differential algebraic equations typically arise as model equations in problems of technical mechanics like robotics or vehicle simulation, or in problems of chemical engineering and reactive flow, e.g. in combustion. In generalization of the forward simulation problem in DAE, optimization boundary value problems have become more and more important in the recent past to solve for complex nonlinear boundary conditions and to optimize performance with respect to energy consumption, product quality, productivity or to minimize unwanted by-products. The talk reports on recent results for parallel optimization algorithms combined with multiple shooting and collocation. In particular, relaxed formulations of index-reduced problems are discussed, which allow for inconsistent initial values and projection on to higher index invariants to improve numerical stability and convergence of the optimization process. Videos with computer animations of parameter estimation in mechanical systems and optimal trajectories for industrial and space robots are shown.

Continuation Methods for Stiff Two–Point Boundary Value Problems

R. Wright and J. Cash

Sequential Regularization Methods for High Index DAE– Equations with or without Singularities

P. Lin and U. Ascher

Two classes of methods have often been studied for the numerical solution of boundary and initial value DAEs: stabilization and regularization. Baumgarte-like stabilization methods (and their various discrete analogues such as coordinate projection and post-stabilization) are popular but are not guaranteed to work well for problems with singularities in the constraints Jacobian. Various regularization methods often yield stiff problems, which probably accounts for their lack of popularity in practice.

We propose a Sequential Regularization Method to overcome both difficulties. We discuss and demonstrate the method for problems with and without singularities, including higher index nonlinear problems.

Continuous Orthonormalization for Two-Point BVPs: Theory and Implementation

E. S. van Vleck

In this talk we revisit the continuous orthonormalization technique for solving two-point boundary value problems and discuss a specific implementation of the method. We show the method is stable by putting it in a multiple shooting-like framework. We present an error analysis for linear problems and an extension to the nonlinear case. Finally, some numerical examples are considered and topics for future work discussed.

The problem of solving two-point boundary value problems (BVPs) for ODEs has received significant attention in the last twenty years. Considerable effort has been paid to the theory and practice for many algorithms, and several reliable, general purpose codes which are suited for many applications have been developed.

Of the various techniques devised for this purpose, global methods (such as collocation) have long been better understood than initial value techniques, and in many respects they appear to have won favor for solving difficult problems. Despite the many desirable features of such methods, for large systems of BVPs the computer power and memory are generally insufficient to allow for their convenient solution. It can be argued that there is great need for more investigation of methods for solving such problems, and indeed, BVPs (stiff or otherwise) have in general received far less attention than the corresponding IVPs. To help resolve some of the questions concerning stability, efficiency and mesh selection for the solution of large systems, IV techniques have been considered as possible alternatives. We propose and analyze an IV-based algorithm which in principle is suitable to handle any type of BVP. It is particularly suited for stiff BVPs, since it retains the same stability characteristics as the BVP itself.

PARALLEL D1: STIFF ODEs

Advanced Steppoint Methods for Stiff and Non-Stiff IVP's

Y. Psihoyios

A class of advanced steppoint methods is developed for the numerical integration of non-stiff systems of ordinary differential equations. These methods lie in between the classes of Adams and explicit Runge- Kuta methods in that they require three function evaluations per step but are implemented in a variable step/variable order predictor-corrector mode. An analysis is given to show how to derive these formulae so that they have accuracy and stability properties which are superior to those of conventional Adams formulae. The new formulae have been implemented in a general purpose variable step & order code and comparisons with the Shampine and Gordon code in the non-stiff DETEST set are given. Finally some important advances in advanced steppoint

methods for stiff problems will also be discussed.

Joint work with J. Cash.

Variable Coefficient Explicit Runge-Kutta Methods for Stiff Equations

M. Nakashima

It is our purpose to propose a class of a variable coefficients explicit Runge-Kutta (abb, R-K) formulae for the numerical integration of stiff equation. The parameters in R-K formulas may be used, for example, to achieve strong damping fitting of the stiff components or to extend stability regions of numerical solutions for some differential equations. Some analysis and numerical examples justifying the results are also given.

The Stability Region and the Accuracy for the Extrapolation Method to I.V.P.in O.D.E.

M. Murofushi and H. Nagasaka

We apply an extrapolation method which can produce a highly accurate numerical solution for I.V.P. in O.D.E.. Our extrapolation method is based on the explicit mid-point rule and Romberg sequences are applied to the inner-stepsize sequence.

Bader and Deuflhard (1983) proposed an extrapolation method based on the semi-implicit mid-point rule. Applying a certain additional smoothing procedure to this method gives A-stability. In view of the stability region and the accuracy of numerical results for Gear's example ($y' = 1000(\exp(x) - y) + \exp(x)$, $y(0) = 1$), we make the following considerations:

1. the comparison between numerical results obtained by Romberg and those obtained by using Harmonic sequences for inner-stepsize ;
2. the comparison between numerical results based on the explicit mid-point rule and those based on the semi-implicit mid-point rule.

From the investigation of these results, we have found that the method based on the Romberg sequences with the semi-implicit mid-point rule is superior.

MVBDF: An Efficient Implementation of Variable Coefficient Backward Differential Formulas

Q. Li, E. K. Blum and Xin Wang

We are motivated to study ODE solvers by our research on simulation of biological neural networks[2]. The realistic compartmental modeling of networks of neurons results in large number (more than 100) of stiff (eigenvalue ratios bigger than 5000), oscillatory (imaginary eigenvalues), and spiking (positive eigenvalues) nonlinear ordinary differential equations. Also, such equations usually have many parameters to be tuned in the process of simulation in order to model biological behaviors of neural networks. Many general purpose integrators (LSODE, VODE, etc.) have been tested on these equations, but are found not satisfactory in many aspects. Among them, efficiency is most important since simulation for modeling purpose usually involves repetitive computation in many times with different sets of parameters. If real-time simulation is a potential application, then the requirement for integration speed is even more stringent.

Considering that one of major computational costs in each integration step comes from solving a large linear system of equations with a coefficient matrix depending on the order of method, step sizes, and the Jacobian of the problem, we design a stable and efficient implementation, MVBDF, of variable coefficient backward differential formulas (BDF) which allows the matrix of the linear system to be kept unchanged as long as possible under the variation of step size and order. The selection of step size and order for the next integration step in MVBDF is controlled by both local error estimation and variation of the matrix of the linear system. Also, by using the divided difference interpolation formula based only on past values, MVBDF is able to vary the current order to any other orders after each integration step stably which is essential for implementing our formulation of maximizing the step size while not incurring more matrix factorization. Compared with variable coefficient BDF solvers EPSODE and VODE[1], MVBDF will have less number of LU-decompositions and integration steps. Numerical experiments on many problems show that MVBDF is an efficient and general ODE solver. When coupled with special techniques in modeling of neural networks, it provides a very useful simulation tool for biological neural networks.

[1] P.N. Brown, G.D. Byrne, and A.C. Hindmarsh, *Vode: A variable-coefficient ode solver*, SIAM J. Sci. Stat. Compt., 10:1038–1051, 1989.

[2] E.K. Blum, Q. Li, S.C.J. Hyland, P.K. Leung, and X. Wang, *BIONNIC: An Efficient and Flexible Integrator for Biological Neural Network Simulators*, Analysis and Modeling of Neural Systems, E.H. Eeckman (ed.) Kluwer Acad. Publ. 1994.

PARALLEL D2: STOCHASTIC DIFFERENTIAL EQUATIONS

Errors in Numerical Approximation of Stochastic Integrals for the Error Analysis in Numerical Simulation of Stochastic Differential Equations

Y. Saito and T. Mitsui

We consider scalar Ito stochastic differential equations (SDEs). A lot of numerical schemes in both strong and weak senses for the SDE are proposed. However, the error of numerical solution has not been clearly analyzed in numerical schemes for SDEs. Thus we have proposed a method of error analysis by separating the global error into two parts (deterministic and stochastic parts). When we analyze the stochastic part, we will have to study that for some basic stochastic integral processes, for example, the Wiener process $W(t)$ and the Wiener integral process $\int W(s)ds$. We applied several numerical schemes, especially weak schemes, for a good approximation of statistical quantities of the solution. The results show that the error depends on the number of trajectories, not on the stepsize, and we will point out some remarks on implementation of numerical schemes.

Generalized Rosenbrock Type Methods for Solving Stiff Systems of Stochastic Differential Equations

S.S. Artemiev

The definition of stiff system of stochastic differential equations with additive and multiplicative noise is introduced. Special family of generalized Rosenbrock type methods is considered. Sufficient conditions of A-stability in the mean - square sence of this family is proved. Also it is introduced the definition of the stability region in the mean - square of a numerical method based on the test scalar Ito SDE

$$dy(t) = (\alpha - \frac{s^2}{2})y(t)dt + sy(t)d\omega(t).$$

The results of numerical experiments obtained with help of the dialogue system "Dynamics and Control" are also presented.

Interactive Solvers for Initial Value Problems for Ordinary and Stochastic Differential Equations

I.O. Shkurko

The power of modern numerical methods for analysis of differential equations would become more accessible for wide range of investigators if methods were involved in the united integrated environment together with user interface in frames of modern information technology. This is especially

actual due to facilities of contemporary computers for which the use of user's interface ("screen windows", "popup menus", mouse, on-line help system, error handler and etc.) is natural. The main advantages of such an integrated environment would be the preparation of initial data for solving problems in easy way, quick choice of appropriate method and its parameters, wide set of functionals and characteristics which can be evaluated for stochastic processes.

In order to eliminate the necessity of coding nonlinear functions by user the internal compiler was designed. The Cauchy problem for ODE and SDE is described by some intuitevely clear script language closed to normal mathematical notation. Several interactive environments based on this approach were developed for IBM PC.

DYNAMICS and CONTROL package solves following problems:

- Linear algebra
- Numerical solution of the Cauchy problem for ODE
- Statistical simulation of solution of the Cauchy problem for SDE and evaluation of different functionals of their solutions
- Minimization of functions of many variables
- Linear and nonlinear filtering on the basis of continuous and discrete, real and model measurements
- Parameter identification for ODE and SDE on the basis of discrete measurements
- Verification of controllability, observability, stability characteristics of linear controlled objects
- Analysis of dynamics of linear controlled deterministic and stochastic objects

RAPSODIE is specialized package for integaration of SDE and ODE with lot of numerical methods and functional evaluations. The possibility of invoving new methods in easy way make the package adaptive for testing different algorithms.

A Convergence Rate Estimation of Runge-Kutta Methods for Numerical Solution of ODE's With Random Right-Hand Sides

O. A. Kurbanmuradov

Let $X(t)$, $0 \le t \le T$ be a solution to the Cauchy problem

$$\frac{dX}{dt} = u(X,t;\omega), X \in R^n, 0 < t \le T, \omega \in \Omega \tag{0.1}$$

$$X(0) = x_0, (|x_0| \le r_0), \tag{0.2}$$

where $u(X,t;\omega)$, $(X,t) \in R^n \times [0,T] = Q_T$ is n-dimentional random field defined on a complete probability space (Ω, F, P). Let

$$\frac{X_{t+h}^{(h)} - X_t^{(h)}}{h} = \Phi_u(X_t^{(h)}, t, h), X_0^{(h)} = x_0 \tag{0.3}$$

be an l-stage Runge-Kutta method for approximate solution of the Cauchy problem and let

$$\varepsilon_{\Phi}^{(h)}(u) = \sup_{x_0:|x_0|\le r_0} \max_{t:0\le t\le T} |X(t_i) - X_{t_i}^{(h)}|, (t_i = ih, i = 0, 1, 2, \ldots) \tag{0.4}$$

be the accuracy of the method. Since $u(X, t; \omega)$ is a random field, $\varepsilon_{\Phi}^{(h)}(u)$ is a random variable too.

The main problem studied is an estimation of the rate of the convergence $\varepsilon_{\Phi}^{(h)}(u) \xrightarrow{P} 0$, as $h \to 0$.

Stochastic Lagrangian Models of Relative Dispersion in Turbulent Flows

K.K. Sabelfeld

There are two main approaches in stochastic modelling of turbulent motion of fluid particles. The first one uses models of Eulerian velocity field $U_E(x, t)$, for instance, randomized Monte Carlo models [1], or models based on numerical methods for solving the Navier–Stokes equation. With such models, one simulates an ensemble of Lagrangian stochastic trajectories and calculates the desired statistical characteristics. Second approach uses different approximations of the Lagrangian velocities of a set of particles. A first model of this type was introduced by G. Taylor in 1921, and then developed by many authors.

The first approach is rigorous, but it requires a lot of computer time. The second is much more effective, but its correct utilization needs special justifications. Both the approaches are useful for modelling the pollutant scattering in turbulent flows, and especially for calculating the concentration fluctuations. Most developed are the one-particle Lagrangian models which allow to calculate only the mean concentration. To find the concentration fluctuations, or, more generally, the covariance of the concentration, it is necessary to have two-particle Lagrangian models. Unfortunately, such models are not well developed.

The motion of two particles can often be regarded as a motion of one particle plus the relative motion of the second particle with respect to the first one. Compared to the absolute diffusion of two particles, it is believed that the relative diffusion can be treated, due to the Kolmogorov's similarity hypotheses, using a simpler and universal description. Therefore, models of relative diffusion attract much attention.

We give here two examples to motivate why the relative diffusion is of particular interest. Assume that we describe a pollutant transport in a homogeneous velocity field, and $c(x, t)$, the instantaneous concentration of the pollutant is also statistically homogeneous. Then $B_c(r, t)$, the covariance of the concentration

$$B_c(r, t) = \langle c(x, t)\, c(x + r, t) \rangle$$

is represented as

$$B_c(r, t) = \int p(r, t|\, r_0) B_c(r_0, 0)\, dr_0. \tag{0.5}$$

Here $p(r, t|\, r_0)$ is the probability density function (p.d.f.)

$$p(r, t|\, r_0) = \langle \delta(r - r_L(t, r_0)) \rangle,$$

where $r_L(t, r_0)$ is the instantaneous separation (at the time instant t) between the particles initially separated by r_0. In derivation of (1) it is supposed that the initial concentration field $c(x, 0)$ is statistically independent of the velocity field.

Thus to evaluate the covariance of concentration it is necessary (and sufficiently, in this case) to know the statistics of the relative motion of two particles.

The second example comes from the Smolouchovsky equation governing the coagulation of particles in homogeneous turbulent flows, where the coagulation rates depend on the relative velocity between two colliding particles.

In this talk we deal with the problem of relative motion of two particles. We suggest different stochastic models (3D and quasi-one-dimensional) which are consistent in a sense with the Eulerian velocity field. We derive new stochastic models in the form of a system of stochastic differential equations. Applications in numerical modelling of the particle dispersion in the atmosphere under the convective conditions are presented.

[1] Sabelfeld K.K. *Monte Carlo Methods in Boundary Value Problems*, Springer-Verlag, New York, Heidelberg, Berlin, 1991.

Wednesday AM

PLENARY SESSION

Implicit Numerical Methods for Stochastic Differential Equations

E. Platen

The talk will give a survey on implicit numerical methods for the strong and weak solution of stochastic differential equations. The stability properties of different algorithms will be discussed with respect to certain classes of test equations.

Stability Analysis of Numerical Solution for Stochastic Differential Equations

T. Mitsui

Linear stability analysis of numerical solution for stochastic differential equations is considered from the viewpoint how it is similar to as well as different from that for ordinary differential equations. Some previous trials for stability concept are arranged.

PARALLEL A: COMPUTING INVARIANT SETS

Heteroclinic Cycles in Load-Coupled Josephson Junctions

E. Doedel

Results of a numerical study of heteroclinic cycles in a model of load-coupled Josephson junctions will be presented and related to results of Terman on the unfolding of a codimension-2 heteroclinic cycle. This is joint work with D. Aronson and D. Terman.

Invariant Manifolds and Global bifurcations for the Kuramoto-Sivashinsky Equation

M. Jolly

We study elements of the global attractor of the Kuramoto-Sivashinsky equation (KSE) in an attempt to classify certain global bifurcation phenomena involving stable and unstable manifolds of steady state and standing wave solutions. These computations are inspired and facilitated by (but not restricted to) the study of a three-dimensional approximate inertial form, for which the phase space can be completely visualized with the help of computer graphics.

On Efficient Computation of Connecting Orbits

M. Friedman

We present recent developments on locating and continuing connecting orbits in ordinary differential equations. We discuss practical implementation issues and give some illustrative numerical examples.

Computing Degenerate Bifurcations

J. Guckenheimer

Many degenerate bifurcations lie on smooth submanifolds in the space of vector fields. We are concerned with algorithms for computing these bifurcations. This lecture will begin with a general discussion of this problem, and then will focus upon recent work of Govaerts, Guckenheimer and Khibnik on the computation of multiple Hopf bifurcations.

An equilibrium point is called a Hopf point if its Jacobian matrix has a conjugate pair of pure imaginary eigenvalues. It is called a double Hopf point if there are two such pairs and a 1:1 resonant double Hopf point if there is a pair of (algebraic) multiplicity two. We describe a method for

numerical detection, computation and continuation of Hopf, double Hopf and 1:1 resonant double Hopf points. A combination of matrix biproduct methods and bordered matrix methods leads to the definition of families of defining functions for these types of points. For double Hopf and 1:1 resonant double Hopf we know of no comparable approaches. We remark that a double Hopf bifurcation is a codimension 2 phenomenon and that a 1:1 resonant double Hopf bifurcation has codimension 3.

We also study the stratified set of Hopf points near a 1:1 resonant double Hopf point in a generic three - parameter unfolding and we draw conclusions for the numerical computation of curves of Hopf points near a resonant point and of the curve of double Hopf points through that resonant point. Our methods extend to the case of more than two Hopf pairs, partly or fully in resonance.

Example computations are done in a fairly realistic and complicated neural model problem with $n = 13$ and $k = 29$. However, to make the methods applicable to large scale problems (e.g. discretized boundary value problems) we reduce the state space to a subspace that contains essentially the generalized eigenspaces of the eigenvalues with largest real part; this is done by a combination of generalized Cayley transforms and subspace iteration. The evidence shows that numerical differentiation in local coordinate systems is accurate enough to allow the numerical treatment of complicated bifurcation points.

PARALLEL B: LINEAR AND NON–LINEAR EQUATIONS

A Preconditioning Method for the Čebyšev Pseudospectral Method

J. Berrut

A preconditioning method for the solution of linear systems arising from applying Čebyšev pseudospectral methods to stationary differential equations is presented. The method avoids the evaluation at each iteration of the spectral differentiation operator of highest order; which usually is the most unstable part of the system.

On the Improved SOR Method with Orderings for Non-Symmetric Matrices

E. Ishiwata and Y. Murayo

We consider the difference equations $Ax = b$ derived from singular purturbation problems. To solve such non-symmetric linear problems, we propose generalized SOR method, named "improved SOR metod with orderings".

For an $n \times n$ matrix A, we choose the proper purmutation matrix P and the relaxation diagonal matrix $\Phi = diag(\omega_1, \cdots, \omega_n)$. Let

$$\tilde{A} = P^T A P, \quad \tilde{x} = P^T x, \quad \tilde{b} = P^T b$$

and $\tilde{A} = \tilde{D} - \tilde{L} - \tilde{U}$, where $\tilde{D}$ is a diagonal matrix, $\tilde{U}$ is an upper triangular matrix and $\tilde{L}$ is a strictly lower triangular matrix.

The improved SOR method with orderings can be expressed as

$$\tilde{x}^{(k+1)} = (\tilde{D} - \Phi\tilde{L})^{-1}\{(I - \Phi)\tilde{D} + \Phi\tilde{U}\}\tilde{x}^{(k)} + (\tilde{D} - \Phi\tilde{L})^{-1}\Phi\tilde{b} \qquad k = 0, 1, 2, \cdots$$

Our method has the following three properties compared with usual SOR method.

- We considered orderings. This is very important point for non-symmetric matrices.
- We changed usefully the relaxation parameters ω_i, $i = 1, \cdots, n$ of Φ.
- $\tilde{U}$ does not always 'strictly' upper triangular matrix.

Our method can be applied to consistently ordered 2-cyclic matrices and its converges so rapidly with few iterations than usual SOR method. We give how to determine the relaxation parameter ω_i, which can be easily determined. Moreover our method can also apply to non-symmetric linear equations derived from singular purturbation problems with turning points. We show convergence theorems and several numerical experiments.

Aspects of the Nonlinear Algebraic Equations in Methods for Stiff ODEs

J. Williams

For the stiff system of m equations

$$y' = f(y), \quad t > 0, \quad y(0) = y_0,$$

the nonlinear algebraic equations which are solved repeatedly in widely used software, such as the implementation of the BDF formulae in LSODE and VODE, take the standard form

$$y_n = h_n \beta_n f(y_n) + \psi_n, \quad \beta_n > 0.$$

For the current step size h_n and known information vector ψ_n, the equations are to be solved for y_n and a modified Newton iteration is often used.

Some results on the existence, uniqueness and error bounds for solutions of these algebraic equations will be briefly described. The possibility of nearly singular Newton correction equations is also considered and illustrated with numerical examples.

Finite-Precision Effects in the Simplified Newton Iteration

R.K. Alexander

Implicit integration formulæ are ordinarily used for the integration of stiff initial value problems. It is normal practice to use a simplified Newton iteration to solve the "algebraic" equations for advancing the computed ODE solution at each step of the integration. This process is fraught with difficulty because the iteration matrix is badly conditioned [2], and because residuals cannot always be evaluated accurately. Consequently, the claim that the simplified Newton iteration is contractive "independent of stiffness" provided only that the integration stepsize is appropriate [1], is too optimistic.

To clarify these issues we consider the class of "badly scaled singular perturbation problems." These are problems which *can* be reduced to singular perturbation form by appropriate scaling of the dependent variables, but are not. Some familiar test problems are posed in exactly this way. Analysis and numerical experiments suggest some refinements to the conclusions of [1] on how to conduct the iteration.

[1] R.K. Alexander, *The modified Newton method in the solution of stiff ordinary differential equations*, Math. Comput. 57 (1991) 673–701.
[2] L.F. Shampine, *Ill-conditioned matrices and the integration of stiff* ODEs, J. Comput. Appl. Math. 48 (1993) 279–292.

The SVD for the Solution of Nearby Polynomial Systems

R.M. Corless, P.M. Gianni, B.M. Trager, and S.M. Watt

This talk discusses singular value decomposition (SVD) algorithms for some standard polynomial computations, in the case where the coefficients are inexact or imperfectly known. We first look at algorithms for univariate polynomial computations (such as GCD), and then explore an adaption of Lazard's algorithm (for the solution of possibly overdetermined homogeneous systems of polynomial equations with a finite number of solutions at infinity) to the inexact-coefficient case. The principal modifications to Lazard's algorithm are to use a generalized eigenvalue computation to simultaneously upper-triangularize a family of commuting matrices instead of forming and then factoring a polynomial determinant, and to use the SVD instead of Gaussian elimination to determine the rank of a generalized Sylvester matrix and hence the number of roots. We discuss the stability and complexity of the algorithms presented here and give examples, including an application of the modified Lazard's method to the location of singular points on projections of algebraic curves.

PARALLEL C1: NUMERICAL METHODS FOR STOCHASTIC DIFFERENTIAL EQUATIONS

Stability Criteria in the Numerical Treatment of Stochastic Differential Equations

R. Spigler

Numerical stability of algorithms for solving ordinary differential equations usually refers to suitable test equations. We consider stochastic differential equations (or systems) of the Ito or Stratonovich type as ordinary differential equations where some Gaussian white noise has been introduced, e.g. to take into account or to model a variety of phenomena. Then we can adopt a similar point of view. In case of systems where only additive noise acts, the analogue of Dahlquist's A-stability of both explicit and implicit Runge-Kutta schemes is considered, and the effect of implicitness upon stability is assessed. It is shown that the discretization of the drift-term alone controls the A-satability of the whole scheme. When the noise acting on the system is multiplicative, a suitable tedt equation is proposed,and (numerical) stability is now intended in a truly probabilistic sense. A class of implicit Runge-Kutta schemes, optimal with respect to the global order ofconvergence in quadratic mean, is obtained, and the corresponding stability regions are given.

On a Method of Numerical Averaging

J. Golec

For stochastic singularly perturbed systems of the form

$$\begin{aligned} dX_t^\epsilon &= b_1(X_t^\epsilon, Y_t^\epsilon)dt + \sigma_1(X_t^\epsilon)dW_t; \qquad X_0 = x_0 \\ dY_t^\epsilon &= \tfrac{1}{\epsilon} b_2(X_t^\epsilon, Y_t^\epsilon)dt + \tfrac{1}{\sqrt{\epsilon}}\sigma_2(X_t^\epsilon, Y_t^\epsilon)dW_t; \qquad Y_0 = y_0 \end{aligned}$$

let us consider the following Euler-type difference scheme:

$$X_{k+1}^h = X_k^h + \frac{h}{N}\sum_{p=0}^{N} b_1(X_k^h, \overline{Y}_k^p) + \sigma_1(X_k^h)\Delta W_k(h); \qquad X_0 = x_0,$$

where

$$\overline{Y}_k^{q+1} = \overline{Y}_k^q + b_2(X_k^h, \overline{Y}_k^q)h + \sigma_2(X_k^h, \overline{Y}_k^q)\Delta\overline{W}_k^q(h)$$

$q = 0, 1, \ldots, N-1$, and $\Delta W_k(h)$, $\Delta\overline{W}_k^q(h)$ are mutually independent $(0, h)$-distributed Gaussian random variables.

We consider the mean-square and the pathwise convergence of X_k^h to the solution $\overline{X}_t$ of the associated reduced problem

$$d\overline{X}_t = \overline{b}(\overline{X}_t)dt + \sigma_1(\overline{X}_t)dW_t; \qquad \overline{X}_0 = x_0,$$

under the existence of an ergodic measure for the original stochastic singularly perturbed system.

PARALLEL C2

The Effect of Stopping the Newton Iteration in the Application of Implicit Linear Multistep Methods

M.N. Spijker

This talk is concerned with linear multistep methods in the numerical solution of stiff initial value problems for systems of strongly nonlinear, ordinary differential equations. The effect of stopping Newton-type iterations in the actual application of linear multistep methods is analysed and related to the stepsize of the methods.

The talk starts by reviewing the local effect of the stopping of the Newton iterations. A theoretical expression for the order of this effect is given along the lines of Dorsselaer & Spijker (1994). The constants in this expression are of moderate size and not affected by stiffness. This theoretical result is confirmed by numerical experiments. Next, the global (accumulated) effect of all local stopping errors is analysed. Numerical experiments show that this effect is of an order which is higher (by one) than what one would expect in view of the estimates of Dorsselaer & Spijker (1994). The rest of the talk deals with attempts to explain this anomaly.

One might be tempted to explain the unexpectedly high order of the global stopping error by some damping effect affecting most of the local stopping errors. But, numerical experiments, pertinent to local and global discretization errors, show that such a damping cannot be present in the situations at hand. A succesful approach to explaining the anomaly mentioned above consists in an application of Hundsdorfer's device (see Hundsdorfer (1992) and Hundsdorfer & Steiniger (1991)). With the help of this device the high order of the global stopping errors will fully be explained along the lines of Spijker (1995).

[1] J.L.M. van Dorsselaer and M.N. Spijker, *The error committed by stopping the Newton iteration in the numerical solution of stiff initial value problems*, IMANA Journ. Numer. Anal. 14, 183–209, 1994

[2] W.H. Hundsdorfer, *Unconditional convergence of some Crank-Nicolson LOD methods for initial-boundary value problems*, Math. Comp. 58, 35–53, 1992

[3] W.H. Hundsdorfer and B.I. Steiniger, *Convergence of linear multistep and one-leg methods for stiff nonlinear initial value problems*, BIT 31, 124–143, 1991

[4] M.N. Spijker, *The effect of the stopping of the Newton iteration in implicit linear multistep methods*, Accepted for publication in APNUM, 1995

PARALLEL D: COMPUTER ALGEBRA TOOLS FOR HANDLING ODEs

CATHODE is the name of an ESPRIT Working Group formed by researchers in several European countries. The name is an acronym for 'Computer Algebra Tools for Handling Ordinary Diffferential Equations', expressing the objective of the working group.
Numerically solving differential equations is a basic procedure in applied mathematics. Though it is often the only feasible method, it is not always what one likes. It will not give information on closed form solutions, if such solutions exist. Neither does it show the dependence on parameters in a functional form. Solutions in closed form and in the form of (asymptotic) series offer more insight in the properties of the solutions than numerical solutions do.
In the last decade computer algebra systems have become mature and computers quick and cheap. This has lead to new possibilities in the research of differential equations by symbolic methods and to computer algebra programs for the study of differential equations.
The ideas, algorithms and programs developed by the various groups in CATHODE are very diverse: closed form solutions, Lie symmetries, series solutions, asymptotics, normal forms,...The talks in this minisymposium illustrate how the algebraic and numerical approaches can complement each other, and concentrate on the aspects of CATHODE which are the most applicable to scientific computation.

Numerical Integration of Dynamical Systems Using Taylor Series

L. Brenig

Early approaches for numerical integration were based on Taylor series. These methods have two major problems. On one hand, it is difficult to compute the general term of the serie. On the other hand, the valuation of its convergence is not an easy task. Other methods have been developed such as Runge-Kutta and finite differences techniques which are now the most commonly used. Recent developments enable us, for a wide class of systems, to obtain a closed form for the general term of the Taylor expansion bringing a renewal of interest for this approach.

More precisely, we study ordinary differential systems of the form :

$$\dot{x}_i = x_i \sum_{i=1}^{n} A_{ij} \prod_{k=1}^{m} {x_k}^{B_{jk}}$$

where A and B are real matrices [1]. This class contains, among others, all polynomial systems. It has been shown [2] that the Taylor expansion for these systems is given in closed form by : $x_i(t) = \sum_{r=0}^{\infty} C_r(i)\, t^r/r!$ where

$$C_r(i) = x_i(0) \sum_{j_1=1}^{m} \cdots \sum_{j_r=1}^{m} A^0_{ij_1}(A^0_{ij_2} + M^0_{j_1 j_2}) \cdots (A^0_{ij_r} + M^0_{j_1 j_r} + \cdots + M^0_{j_{r-1} j_r}),$$

$$A^0_{ij} \equiv A_{ij} \prod_{k=1}^{n} x_k(0)^{B_{jk}}, \quad M^0_{ij} \equiv M_{ij} \prod_{k=1}^{n} x_k(0)^{B_{jk}},$$

$M \equiv B \cdot A$ and $x(0)$ represents the initial condition.

Using this, we can develop new techniques, we would like to compare with standard ones (Runge-Kutta). This comparaison should be done also in the regions with a high sensibility to initial conditions. Some advantages of techniques using Taylor expansion are

- A good estimation of the error given by the rest of the serie.
- An accuracy control process increasing the order of truncation rather than reducing the step size of integration.

[1] A. Goriely and L. Brenig, *Phys. Let. A145*, (1990) p. 245
[2] L. Brenig and A. Goriely, *Painlevé Analysis and Normal forms*,in Computer Algebra and Differential Equations, edited by E. Tournier, Cambridge University Press, pp 211-238.

Computer algebra methods for solving ODE (A survey of the DESIR II project)

V. Gilles

The DESIR II project has as a (far reaching) goal the construction of computer algebra tools for the integration of (systems of) ODE. The point of view is that we must be able to first classify systems using computer algebra methods, and then build special algorithms for general classes of problems. Following this way we have started by a library of programs for *(formal) linear algebra* (normals forms of matrices including Frobenius, Smith, Jordan...) and their applications to the linear differential problem with constant coefficients ($X' = AX$). Then we have implemented algorithms for ODE systems with singularities ($X' = A(x)X/x^q$). Another direction of research is dedicated to normal forms problems for ODE and DAE. Severals results (using computer algebra tools) will be presented.

Plan: Formal linear algebra, ODE with singularities, normal forms for ODE and DAE.

A Symbolic Calculus for Higher Order Derivations and Geometrically Stable Integration Algorithms for Rigid Bodies

R. Grossman

Let G denote a finite dimensional algebraic group, R its coordinate ring, g its Lie algebra, and $Y_1, \ldots, Y_N$ a basis for g. In this talk, we describe a symbolic calculus for higher order derications on G. We then apply this calculus to derive numeric and symbolic algorithms to solve differential equations on G of the the form:

$$\dot{x}(t) = F(x(t)), \qquad x(0) = p \in G,$$

where

$$F = \sum_{\mu=1}^{N} a^{\mu} Y_{\mu}, \quad a^{\mu} \in R$$

is a vector field on G.

Our main examples are the rotation group and Euclidean group in three space. We give examples of how these algorithms apply to rotating rigid bodies and to rolling balls on planes.

The numerical algorithms we develop and analyze are *geometrically stable* in the sense that if x_n is the approximation to the trajectory $t \to x(t)$ at time t_n, and if x_n lies in the group G, then, except for round-off error, the next iterate x_{n+1} also lies in the group G. Generally, numerical algorithms have the property that by the structure of the algorithm itself approximation errors are introduced with the consequence that x_{n+1} is not on the group G. The algorithms we analyze have the further property that if G is the abelian group $\mathbf{R}^N$, then the algorithms reduce to classical single and multi-step algorithms.

The basic idea is to introduce a data structure involving trees to code the effect of higher order versions of Leibntz's rule, and then to exploit the natural algebraic structure of trees in order to derive the algorithms.

This talk is joint work with Peter Crouch and Richard Larson.

Wednesday PM

PLENARY SESSION

How Can We Simulate Motion of Large Biological Molecules ?

T. Schlick

Many problems in chemistry can be reduced to the solution of systems of coupled ODEs. Examples include molecular dynamics (MD), rate equations of kinetic theory, and the time-dependent Schrödinger equation when expanded in a basis set. The technology of numerical integrators for solving ODE's has a long history with significant interplay between mathematics, physics and chemistry. Many of the earliest integrators, such as Runge-Kutta and predictor-corrector integrators, are still in common use, but there have also been recent advances, driven by the need for methods that can treat multiple timescales and have greater stability for the large-scale, coupled nonlinear oscillators commonly found in MD of polymers and biological macromolecules. The long-time stability of integrators for such complex, often chaotic, systems is a challenging area of mathematical-analysis research, and perhaps the context of biomolecular MD will stimulate important developments.

In MD, molecular motion is propagated by numerically integrating the classical equations of motion. The governing force field is constructed semi-empirically. In theory, MD simulations can provide extensive spatial and temporal information, but inadequate sampling limits the scope of the results that can be obtained in practice. Standard explicit schemes, while simple to propagate and modest in memory requirements, impose a severe constraint on the maximum timestep possible (around 1 fs = 10^{-15} s). This value is determined by the period associated with high-frequency modes (e.g., bond stretches), and it contrasts the much longer timescales (up to 10^2 s) which govern key configurational changes in macromolecules (e.g., folding).

Standard techniques of effectively freezing the fast vibrational modes by a constrained formulation increase the timestep by a small factor, still with added complexity at each step. The multiple-timestep approaches for updating the slow and fast forces provide additional speedup, but stability issues have been noted. Standard implicit techniques for stiff ODEs are not directly applicable to MD of macromolecules because: (i) Suppressing the rapidly-decaying component of the motion alters the dynamics because of the intricate vibrational coupling and energy transfer involved. (ii) Schemes with numerical damping (e.g., implicit-Euler) can lead to unphysical results, even when energy-restoring mechanisms are used. (iii) The increased complexity (e.g., solving a nonlinear system) requires significant timestep increases for competitiveness with "brute-force" integrations. One possible approach to these problems is to construct a separating framework for the fast and slow motions. For example, a combination of normal-mode techniques with implicit integration can resolve the high-frequency and low-frequency motions by techniques adequate for

each regime[1,2]. Such ideas for MD, and others, will be presented and discussed, with emphasis placed on new research directions.

[1] G. Zhang and T. Schlick *LIN: A New Algorithm to Simulate the Dynamics of Biomolecules by Combining Implicit-Integration and Normal Mode Techniques*, J. Comp. Chem., **14**, 1212–1233 (1993).
[2] G. Zhang and T. Schlick, *The Langevin/Implicit-Euler/Normal-Mode Scheme ("LIN") for Molecular Dynamics at Large Time Steps*, J. Chem. Phys., **101**, 4995–5012 (1994).

Thursday AM

PLENARY SESSION

Classical Accelerators for Waveform Relaxation Methods with Application to Parallel Solution of ODE's

J. White

The standard approach to solving ODE's generated by spatial discretization of time-dependent partial differential equations is to apply implicit integration methods. Then, the generated sequence of algebraic equations are solved using Newton's method combined with a Krylov-subspace based iterative matrix solution method. Such an approach is difficult to parallelize on loosely coupled parallel processors because of the frequent synchonization required. Waveform relaxation (WR) methods offer an appealing alternative because the waveform-based decomposition has significantly fewer synchronization points. However, WR methods can converge very slowly, and theoretical results indicate that classical SOR and Krylov-subspace based techniques provide limited acceleration. In this talk, we present an extension to SOR, convolution SOR, and give some optimality results to show that convolution SOR is as effective an accelerator. In addition, we present a different approach to examining Krylov-subspace methods to show why they are more effective in practice than expected. Finally, we present computational results from solving the nonlinear time-dependent drift-diffusion equations generated by semiconductor device simulation problems. Results are given which demonstrate that the waveform methods perform much better on loosely coupled parallel processors than standard techniques.

Shadowing in Chaotic Systems

C. Grebogi

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. I will also discuss the complications that arise in higher dimensional systems when some of the Lyapunov exponents associated with a given numerical trajectory are close to zero.

PARALLEL A: SHADOWING

Much can be learned about the dynamics of a specific dynamical system through computer experiments. However, the reliability of numerical simulations of dynamical systems, especially chaotic ones, remains a major concern. Shadowing is the technique of rigorously establishing true solutions nearby a locally well-behaved approximate solution. Professor Kloeden will discuss shadowing in forward and backward directions for semi-hyperbolic discrete dynamical systems. Professor Palmer will present results for rigorously establishing the existence of periodic solutions from numerically computed approximate periodic solutions of maps and ordinary differential equations. Professor Eirola will discuss shadowing numerical solutions of parabolic partial differential equations.

Bi-Shadowing in Semi-Hyperbolic Dynamical Systems

P. Kloeden

A concept of bi–shadowing is introduced for discrete–time dynamical systems. It combines the usual direct shadowing of a pseudo–trajectory by a true trajectory with the inverse shadowing of a true trajectory by a pseudo–trajectory of a nearby system belonging to some prescribed class of systems. It is shown that the semi–hyperbolicity of the mapping generating the system implies that it is bi–shadowing. Semi–hyperbolicity is a generalization of hyperbolicity to Lipschitz mappings that need not be invertible or smooth. Its definition includes explicit bounds for rates of expansion or contraction and leakage from the splitting subspaces that are invariant in the hyperbolic case.

These results are based on joint work with Phil Diamond, Viktor Kozyakin and Alexei Pokrovskii which has been funded by the Australian Research council grant A 8913 2609.

Computation of Periodic Orbits in Chaotic Dynamical Systems

K. J. Palmer

Much can be learned about chaotic dynamical systems from their periodic orbits. This talk, which describes joint work with Brian Coomes and Huseyin Kocak, gives a Newton type algorithm for the computation of stable and unstable periodic orbits of high periods for both maps and ordinary differential equations. Also a method, based on shadowing, is given for rigorously verifying that one of these numerically computed orbits approximates a true periodic orbit. The computation of Floquet exponents will be discussed also.

Pseudotrajectories Generated by a Discretization of a Parabolic Equation

T. Eirola and S. Pilyugin

A semi–implicit discretization of the one–dimensional parabolic equation $\partial_t u = \partial_x^2 u + f(u)$ with Dirichlet boundary conditions is considered. Under suitable assumptions on f this defines a C^1–diffeomorphism ϕ of $\mathbf{R}^N$, where N is the number of space grid points. First it is shown that ϕ is dissipative and that the Hausdorff dimensions of its compact invariant sets are bounded uniformly with respect to the space and time

discretization steps. Similar results for other discretizations can be found in the literature. Then the main new result states that for a C^p–generic f ϕ is a Morse–Smale diffeomorphism. Then pseudotrajectories of ϕ are considered. These are ones that are locally close to trajectories of ϕ, i.e., at each step a small error is introduced. It is shown that any attractor of ϕ is approximated well by unions of ω–type sets of any complete family of pseudotrajectories. Also it is shown that for generic f (of those satisfying other assumptions) the pseudotrajectories are Lipschitz–shadowed by trajectories of ϕ. Also connections to the trajectories and attractors of the semigroup generated by the original parabolic equation are discussed.

PARALLEL B: WAVEFORM RELAXATION

Classical Accelerators for Waveform Relaxation Methods with Application to Parallel Solution of ODE's

M. Reichelt, A. Lumsdaine, and J. White

The standard approach to solving ODE's generated by spatial discretization of time-dependent partial differential equations is to apply implicit integration methods. Then, the generated sequence of algebraic equations are solved using Newton's method combined with a Krylov-subspace based iterative matrix solution method. Such an approach is difficult to parallelize on loosely coupled parallel processors because of the frequent synchonization required. Waveform relaxation (WR) methods offer an appealing alternative because the waveform-based decomposition has significantly fewer synchronization points. However, WR methods can converge very slowly, and theoretical results indicate that classical SOR and Krylov-subspace based techniques provide limited acceleration. In this talk, we present an extension to SOR, convolution SOR, and give some optimality results to show that convolution SOR is as effective an accelerator. In addition, we present a different approach to examining Krylov-subspace methods to show why they are more effective in practice than expected. Finally, we present computational results from solving the nonlinear time-dependent drift-diffusion equations generated by semiconductor device simulation problems. Results are given which demonstrate that the waveform methods perform much better on loosely coupled parallel processors than standard techniques.

Waveform Relaxation Acceleration via Time Mesh Coarsening

B. Leimkuhler[1]

Dynamic iteration schemes (waveform relaxation methods) offer a flexible tool for obtaining parallel speedup in the numerical solution of time dependent partial differential equations. For example, varying the time window size or the choice of splitting can allow the schemes to be adapted to a particular architecture or to a given class of problems. Yet dynamic iterations have still not found widespread use as a scientific computing tool.

[1]This work was supported by NSF grant DMS-9303223

Part of the problem is the lack of suitable algorithms and codes. For example, the determination of proper window size, estimates for convergence rate, selection of splitting, and the development of good, portable software are all still open problems, despite some recent progress. Another difficulty is that these methods, like the related stationary iterative methods long used for algebraic systems, often converge very slowly. This behavior is especially noticeable when the problems posess multiple scales, since it is typically necessary to resolve the solution on a fine time mesh in order to have any accuracy in the observable quantities of interest. This is the case in most nonlinear problems, but also for time dependent linear systems such as the Schrödinger equation.

Even if the solution must ultimately be computed on a fine time mesh, it is natural to ask whether it might not be possible to utilize course time mesh approximations at an intermediate stage of the iterative process. In particular, it is natural to ask if the defect in an intermediate fine-mesh approximation can be resolved partially using a course mesh version of the discretized problem. In this way, one is led to acceleration schemes based on time-mesh coarsening, as well as, ultimately, to multigrid-in-time methods. (Note that these methods differ fundamentally from waveform relaxation schemes for parabolic equations based on multiple spatial discretizations, although the analytical methods used to study spatial multigrid waveform relaxation are applicable here.)

In this talk, I will describe some of the problems involved in using these multiple time mesh accelerations. I will focus primarily on a model linear wave equation. The convergence behavior of the scheme is determined by that of the underlying iterative method, the coarsening strategy used, and the properties of the discretization scheme. A few general theorems can be formulated, and model problem analyses are also possible; I will give examples of each. Numerical experiments with both linear and nonlinear problems will also be described.

Multigrid Waveform Relaxation for Parabolic PDEs

S. Vandewalle

Multigrid waveform relaxation is a rapidly convergent, highly parallel iterative method for solving systems of ordinary differential equations obtained by spatial discretization of parabolic PDEs. In this talk I will survey some recent developments.

In the first part of this talk I will outline the theoretical convergence framework for systems of the form $B\dot{u} + Au = f$, obtained after a spatial discretization based on finite elements. This framework will be used to study the method's convergence for isotropic and anisotropic parabolic PDEs. The effect of different waveform smoothers will be analyzed. In the second part of the talk, I will show how the discrete-time multigrid waveform relaxation method can be interpreted as a classical multigrid method on a grid extending in space and time. Hence, classical multigrid analysis tools can be employed to predict accurate convergence rates. The identification with a standard multigrid method also allows one to develop variations to the method, that are no longer based on waveform relaxation. Finally, I will discuss the complexity of the method, and illustrate its poly-logarithmic parallel complexity by timing results obtained on a Connection Machine.

PARALLEL C: DIFFERENTIAL ALGEBRAIC EQUATIONS

DAIs - Differential Systems with Inequality Constraints

U.M. Ascher

While DAEs - differential systems with algebraic equality constraints - have been frequently considered in the literature, resulting in relatively satisfactory theory and efficient algorithms being known, the case for algebraic inequality constraints has rarely been considered and much less is known about it. And yet, DAIs frequently arise in practice. For instance, a physical system whose dynamics is described by an ODE would often have additional nonnegativity requirements on its variables. Such additional requirements would form an inequality invariant. Another example is given by a robot whose motion is required to obey various inequality constraints. The task is to locally plan and control the robot's motion, respecting the constraints as well as Newton's second law. A third example is moving meshes in time-dependent PDE integration, where the mesh points are required to obey constraints like not crossing one another.

One purpose of this talk is to present a perspective on DAIs in general terms. We then concentrate more on problems of local control, and describe algorithms which are based on a 'least constraint' principle. This means that rather than hanging on to the boundary of the feasibility region (as active set algorithms do), least constraint algorithms attempt to choose a trajectory which stays away as much as possible from all constraints. This can be achieved using a barrier method with local planning. Together with R. Spiteri and D. Pai we have developed such algorithms, and I will describe and demonstrate their performance.

PIRK Methods for Index 2 and Index 3 DAE BVPs

I. Gladwell and K. Woodson

COLDAE uses PIRK methods in a general purpose code for solving Hessenberg index 2 differential algebraic boundary value problems. We extend the code and the analysis in two directions: to a more general class of index 2 problems and to Hesssenberg index 3 problems. In both cases we make the extension without changing the type of information which the user must already supply to the current COLDAE code.

Discontinuous Solutions and Stable Operating Points of Nonlinear Circuits

W.C. Rheinboldt

It is well known that the differential-algebraic equations (DAEs) modeling nonlinear circuits may possess discontinuous solutions. Recently, a general theory of discontinuous solutions of semilinear DAEs has been developed in the setting of distributions (Rabier and Rheinboldt, 1994a/b). In particular, the theory showed that uniqueness of solutions of initial value problems breaks down completely in the class of discontinuous solutions. This leads to the question of finding selection criteria for solutions that correspond, say, to physically acceptable ones. One such (mathematical) selection procedure was given in the second part of the mentioned paper. It involves the perturbation of the original DAE into a socalled completely

nonsingular DAE which possesses only classical solutions and then utilizes a type of consistency condition to characterize the acceptable solutions.

The results have been applied to various nonlinear circuit problems. In particular, the selection procedure has shown itself to agree fully with the known physical reality for these circuits. Moreover, the mentioned consistency condition turns out to be closely related to some of the stability considerations used for operating points of such circuits. A summary of the relevant results and of the connections with stable operating points will be given. In addition, it will be shown that for certain types of circuits, especially those with higher dimensional manifolds of operating points, the solution behavior may show very unusual features.

Numerical Solution of Highly Oscillatory Multibody Dynamic Systems

J. Yen and L.R. Petzold

Numerical solution of differential-algebraic equations that arise from multibody dynamic systems may exhibit low-amplitude but highly oscillatory behavior during the simulation. In many cases, we may not be interested in these oscillations, which are coupled with the slow varying solutions. The convientional numerical methods for DAE may become inefficient since they should resolve the oscillatory solutions using very small stepsize. For the reason of a fast simulation, an efficient solution of this class of problems is desirable, specially, of large-scale systems, such as ground vehicle models.

We consider the multibody systems formulated as ODE with invariants, where stiff forces and torques are the sources of high oscillation in the solution. A family of projection operators, using *coordinate-spliting* technique, is derived to obtain a local *implicit state-space form* of the original problem. Apply linear multistep numerical integration methods to the resulting DAE, the iterative solution can be obtained using an effective Newton-type method, abreviated CM, of which the iterations can filter out high oscillation in some coordinates. A convergence result of the proposed CM method will be presented. The numerical example of a highly oscillatory *bushing* force applied to a two-body pendulum will be used to illustrate the effectiveness of this method.

PARALLEL D: HAMILTONIAN SYSTEMS

Numerical Aspects of Isospectral Flows

M.P. Calvo

In the last years there has been a growing interest in studying methods for the numerical integration of systems of ordinary differential equations that preserve some characteristic properties of the exact flow of the system. An instance of such methods are the well known *symplectic* integrators which preserve the symplectic structure of phase space for Hamiltonian symtems. A second example, that will be considered in this talk, are *isospectral* methods.

We are interested in the numerical integration of differential equations of the form

$$\begin{aligned} \frac{d}{dt}A(t) &= [B(A(t)), A(t)], \quad t \geq 0 \\ A(0) &= A_0, \end{aligned} \tag{0.6}$$

where $[\cdot,\cdot]$ denotes the conmutator of two matrices, A is a $d \times d$ real matrix, A_0 is a symmetric matrix and B is a matrix function in such a way that $B(A)$ is a $d \times d$ skewsymmetric matrix. It is well known that the solution of (0.6) can be obtained by solving the system

$$\begin{aligned} \frac{d}{dt}U(t) &= B(A(t))U(t), \quad t \geq 0 \\ U(0) &= Id \end{aligned} \tag{0.7}$$

and using the relation $A(t) = U(t)A_0(U(t))^T, \quad t \geq 0$. As the solution $U(t)$ of (0.7) is an orthogonal matrix, $\sigma(A(t)) \equiv \sigma(A_0)$ (i.e. the flow of (0.6) is *isospectral*). Numerical integrators for which the associated numerical flow also preserves the spectrum of the solution of (0.6) are called *isospectral* methods.

We present *isospectral* methods of orders 2 and 4 for the numerical integration of (0.6) and analyze the convergence of these methods. Since (0.6) can be viewed as a Hamiltonian system (Toda lattice equations) it can be then efficiently integrated using symplectic methods. Numerical experiments are also presented for the particular case where the solution of (0.6) is related with the QR iteration for approximating the spectrum of a symmetric matrix.

Structure-Preserving Integrators and DAEs

L.O. Jay

We are concerned with the numerical solution of Hamiltonian and mechanical systems with holonomic constraints. Such problems arise, e.g., in the modelling of multibody systems and of molecular processes. We present a class of methods based on Lobatto points which preserve (or quasi-preserve) certain features of the flow: symplecticity, reversibility, the manifold of constraints, and energy. These methods are the s-stage (partitioned Runge-Kutta) PRK methods Lobatto IIIA-IIIB. For separable Hamiltonians of the form $H(q,p) = \frac{1}{2}p^T M^{-1} p + U(q)$ the two-stage method is equivalent to the Verlet-Rattle scheme. Structure-preserving methods are of interest for the long-time integration. Some issues related to a reversible variable-stepsize implementation will be briefly discussed. For stiff oscillatory problems, e.g., for the simple stiff spring pendulum equations, the concept of (periodic) P-stability is of importance. For non P-stable methods, such as the Lobatto IIIA-IIIB pairs, the stepsizes are restricted by stiffness. As a remedy, in order to take large stepsizes in case of negligible oscillations, we propose a modification of the Lobatto IIIA-IIIB pairs leading to P-stable methods.

Symplectic Integration of Constrained Hamiltonian Systems: Two Applications

E. Barth

In molecular dynamics simulations, molecules are typically modeled as a system of atomic particles interacting in a potential field which depends only on the position of the atoms. The resulting Newtonian equations of motion are a Hamiltonian system. An explicit numerical integration scheme for this system, commonly used in molecular dynamics, has been shown to be symplectic. To a large extent, long timescale

molecular motion of biological interest has proven difficult to simulate with explicit integration schemes; the fastest components of the potential restrict the stability and hence the size of timestep. One treatment of this problem replaces the fast components with algebraic constraints. A constrained discretization scheme for the resulting system, which has long been popular in the molecular dynamics community, has been shown to be symplectic. We briefly discuss our recent work on efficient treatment of the nonlinear equations resulting from constraints.

Through a particle representation first presented by Routh (1905), a rigid body can be modeled as a rigid molecule— a simple collection of massive particles and quadratic length constraints— preserving its dynamical properties. By way of a slightly generalized particle modeling procedure, which we call *particulation*, we have applied the symplectic constrained techniques from molecular dynamics to conservative multibody systems. Systems of rigid bodies can be readily treated with this technique, with mechanical joints between bodies modeled by quadratic length-type constraints.

Numerical Integration of Constrained Hamiltonian Systems with Application to Molecular Dynamics Simulations

S. Reich

In the first part of our talk we will report about recent result on the numerical integration of constrained Hamiltonian systems. The focus is on methods that preserve the symplectic structure of the flow and/or first integrals due to the invariance of the Hamiltonian under certain symmetry groups.

As an application we consider in the second part of our talk Hamiltonian systems that arise in the context of molecular dynamics (MD) simulations. Such systems are characterized by the presence of highly oscillatory components that arise from the bond stretching and bond-angle bending potentials. Since the presence of these highly oscillatory components forces any explicit integrator to use a very small step-size, the numerical integration of such systems provides a challenging task. It has been suggested previously to replace the strong potentials by holonomic constraints that force the solutions to stay at the equilibrium value of the corresponding potential. This approach has, e.g., been successfully applied to the bond stretching in MD simulations. In other cases, such as the bond-angle bending, this method fails due to the introduced rigidity. Here we suggest instead a constrained formulation that maintains the flexibility of the system while at the same time suppressing the high-frequency components in the solutions and thus allowing for larger time steps in the numerical integration. The new constrained formulation is Hamiltonian and can be discretized by the methods discussed in the first part of the talk.

Applications of Symplectic Integrators to Classical and Quantum Dynamics Simulations

S.K. Gray

The suitability of a variety of explicit symplectic integrators (SIs) to carry out both classical and quantum dynamics simulations is addressed. The SIs employed are those originally devised by Ruth, Candy and Rozmus, McLachlan and Atela, and Calvo and Sanz-Serna, which are particularly suited to large-scale simulations.

As is well known, symplectic integrators may be used to generate numerical solutions to systems of Hamiltonian ordinary differential equations. It is shown how certain SIs can yield very accurate and efficient

results for a classical molecular dynamics simulation of a 1000 unit polymer problem. (The various methods are also tested in relation to a simple, analytically solvable problem.)

Quantum dynamics in both its time-dependent and time-independent forms can also be cast into a (usually large) system of Hamiltonian ordinary differential equations, and it is shown how SIs can be used to provide very efficient means of generating certain quantum mechanical simulations. Regarding the time-dependent Schroedinger equation, it is shown how certain SIs provide high quality short-time approximations to the propagator that should be of particular use in very large problems because of the small memory requirements and ease of programming. Finally, SIs are applied to the solution of the coupled channel equations of (time-independent) inelastic scattering theory. In this case, it is found that SIs will be of relevance when very high accuracy transition probabilities (or S-matrix elements) are required.

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Thursday PM

PLENARY SESSION

On Some New Achievements of the Researchers in the Former Soviet Union in Numerical Solution of ODE and DAE

S. S. Filippov

A brief survey of methods and applications includes the following items:

- Multistep formulas, including formulas with second derivatives,
- Local linearization method,
- Singularly perturbed equations and DAE,
- Runge-Kutta methods,
- Solving stiff equations with explicit methods,
- Nonlinear methods.

Efforts aimed to improve stability and accuracy of the existing linear multistep methods (LMM) were made by several authors. Gerasimov and Kulchitskaya (Moscow) suggested two approaches for optimizing LMM and generalized Gear's algorithms for solving explicit and implicit equations. They developed also a code for solving delay differential equations. Zolotukhin (Kiev) suggested other way to optimize properties of LMM. He produced two codes, GEARZ and GENRZ, which proved to be more effective than codes based on BDF formulas and Enright's method with second derivatives, respectively. The codes mentioned above were successively used for solving of a number of applied problems, such as radiation induced conductivity of polymers, nucleosynthesis in nature, landing of an aircraft, highly oscillatory electrical discharge in gases, etc.

A new development of the method of local linearization for solving stiff equations with instabilities in chemical kinetics is given by Pavlov and Rodionova (Moscow). The numerical scheme is derived from the basic integral equation of the method. This method allows one to study numerically such phenomena as bursts etc.

Different aspects of numerical integration of DAE and singularly perturbed equations were studied by Boyarintsev and his collaborators Chistyakov and Danilov in Irkutsk. Major attention was paid to the theory for linear systems, but implemented algorithms are also capable to cope with nonlinear equations.

It is impossible to give a scope of the extensive studies in one-step methods in a brief survey. So I shall confine myself to the theory of Runge-Kutta methods developed by Kuznetsov (Novosibirsk). Using his

techniques of trial functions and the principle of the weak approximation he derived the fundamental equations of Runge-Kutta methods in a quite simple way. Furthermore, he revealed the importance of nilpotential and completeness properties of Butcher's matrices and developed an unified algebraic theory of explicit, DIRK, and SDIRK methods.

Several schemes for solving stiff problems derived by Lebedev (Moscow) use very simple explicit formulas with embedded parameters on each step, but peculiar sequences of step sizes and parameter values are needed to ensure stability and accuracy of his method. The construction of these sequences is based on the properties of Chebyshev polynomials. Other approaches were developed by Rakitskii (Sankt Peterburg) and Novicov (Novosibirsk).

Nonlinear methods were studied by the groups in L'viv (Ukraine) and Mensk (Belarus'). Basically, Bodnarchuk, Slonevskii, and others in L'viv employed consistently the idea of approximating solutions of ODE by rational functions. Both one-step and multistep methods were developed, implemented, and used in practice. Bobkov and his collaborators in Mensk put forward another approach; it is based on introducing a regularization factor. Unusual nonlinear methods were constructed by Suris (Sankt Peterburg) for some special classes of ODE.

Adaptive Methods for Differential Equations

C. Johnson

We give a survey of joint work with K. Eriksson, D. Estep and P. Hansbo on adaptive quantitative error control for computational methods for differential equations. We present a framework for design and analysis of reliable and efficient methods for adaptive error control and present applications to a variety of dynamical systems.

[1] K. Eriksson, D. Estep, P. Hansbo and C. Johnson, *Adaptive Finite Element Methods*, North Holland, to appear.

[2] K. Eriksson, D. Estep, P. Hansbo and C. Johnson, *Introduction to Adaptive Methods for Differential Equations*, Acta Numerica, to appear 95.

[3] K. Eriksson, D. Estep, P. Hansbo and C. Johnson, *Introduction to Numerical Methods for Differential Equations, Oxford Press, to appear 95.*

PARALLEL A: PARTIAL DIFFERENTIAL EQUATIONS

Convergence Rates for Irregular Meshes

A. Wathen and P. Selwood

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

In this talk we consider irregular grids in the context of refinement paths, i.e. sequences of grids such that $h \to 0$. For a two-point bundary value problem with piecewise linear finite elements for which $O(h^2)$ convergence is expected in the L_2 sense, we will demonstrate a family of grids that give $\|u - u_h\| \leq Ch^p$ where p can take any value in the interval $[2, 2.5)$. Here, as usual, h is the maximal mesh size and u and u_h are the actual and approximate solutions. Despite this apparent superconvergence, these grids actually define a sub-optimal refinement path. This is due to the high degree of irregularity of the meshes.

We will go on to show more practical mesh strategies deriving from the common technique of equidistribution which do not give rise to quasi-uniform meshes even for simple problems. It will be shown that unusual convergence rates can be obtained even in these more practical cases. Asymptotic descriptions of errors in terms of 'mesh functions' and the number of degrees of freedom in an approximation are also possible and we will discuss conditions under which the different descriptions are equivalent, and conditions under which they can be (markedly) different.

Computation of FEM Solutions for Semi-Linear Elliptic PDEs on Large 3D Grids

T. Humphries

We solve parameterized semi-linear elliptic PDEs in 3D, of the form $\Delta u + f(u; \lambda) = 0$, using the finite element method with path following on an SGI work station. This requires the solution of a large system of nonlinear FEM equations at each step of the path following. On small grids this can be accomplished by a Newton-Raphson iteration using using the Conjugate Gradient method to solve the linear update equations with the Jacobian as coefficient matrix. However this approach requires storage of both the stiffness matrix (which is a discrete representation of the Laplacian operator) and a Jacobian matrix. On large grids ($\approx 10^6$ nodes) this is infeasible, even with a sparse element-matrix representation. We describe a quasi-Newton method, applicable to quasi-regular grids (meaning many of the elements have the same shape) for solving these nonlinear equations. One of the main features of this implementation is that the Jacobian matrix is regarded as the stiffness matrix plus a correction due to the nonlinear terms, and that if the solution 'u' is smooth and $|f(u; \lambda)| \gg |u|$ then the 'nonlinear' part of the Jacobian can be diagonalized by 'lumping' all the terms onto the diagonal. This method performs well, retaining the quadratic convergence of the Newton iteration, whilst the assumptions on 'u' and 'f' hold. We show how it can be further modified by retaining some nonlinear element matrices to obtain solutions when 'u' is forming a point singularity

and/or $|f(u,\lambda)| \gg |u|$ on a small section of the domain, again retaining the fast convergence of the Newton iteration. This method has been used to detect the formation of point singularities (under variation of the parameter λ) in semi-linear elliptic PDEs nonlinearities which grow at least as fast as the critical Sobolev exponent, and we present these results.

New NAG Library Software for the Numerical Solution of 1-D Convection-Diffusion Equations

V. Pennington and M. Berzins

New NAG Fortran Library routines are presented for the numerical solution of systems of non-linear, time-dependent convection-diffusion equations in one space dimension, with optional source terms. Convection terms are discretized using a MUSCL-type upwind scheme based on the user-supplied solution of a Riemann problem at each mesh point.

The routines have a method-of-lines structure, and there is scope for coupled ordinary differential or algebraic equations, and adaptive spatial remeshing. The underlying time integration software is shared with existing PDE routines in the Library (employing finite differences, Keller box and C0 collocation schemes), and provides robust and powerful differential-algebraic equation capabilities. Results are presented for standard and non-standard examples, demonstrating the physically realistic solutions obtainable for a broad and challenging class of problems.

[1] Pennington, S.V. and Berzins, M., *New NAG Library software for first-order partial differential equations*, ACM Trans. Math. Software, **20(1)** pp. 63–99 (1994).

Convolution SOR Waveform Relaxation for Parabolic PDEs: a Theoretical and a Model Problem Analysis

J. Janssen

The continuous-time convolution SOR waveform relaxation algorithm for systems of ordinary differential equations of the form

$$B\dot{u} + Au = f\ , \quad u(0) = u_0\ , \tag{0.8}$$

obtained after finite element discretisation of a parabolic partial differential equation, is a straightforward extension of the algorithm in [1]. It consists of two steps, i.e.,

$$\left(D_B\frac{d}{dt} + D_A\right)\hat{u}^{(\nu)}(t) = \left(L_B\frac{d}{dt} + L_A\right)u^{(\nu)}(t) + \left(U_B\frac{d}{dt} + U_A\right)u^{(\nu-1)}(t) + f(t)\ , \tag{0.9}$$

and

$$u^{(\nu)}(t) = u^{(\nu-1)}(t) + \int_0^t \omega(\tau)\cdot\left(\hat{u}^{(\nu)}(t-\tau) - u^{(\nu-1)}(t-\tau)\right)d\tau\ , \tag{0.10}$$

where $B = D_B - L_B - U_B$ and $A = D_A - L_A - U_A$, with D_B and D_A diagonal, L_B and L_A lower triangular and U_B and U_A upper triangular matrices. Note that the difference with standard SOR waveform relaxation is the convolution with a time-dependent SOR kernel $\omega(t)$ instead of multiplication with a scalar ω in the second step of the algorithm.

In this talk, a theoretical framework to investigate the convergence properties of the method is developed. Therefore, the iterative scheme (0.9)–(0.10) is rewritten in explicit form, i.e.,

$$u^{(\nu)} = \mathcal{K}^{CSOR} u^{(\nu-1)} + \varphi \,, \tag{0.11}$$

with $\mathcal{K}^{CSOR}$ the continuous-time convolution SOR waveform relaxation operator. In particular, I shall prove an expression for the spectral radius $\rho(\mathcal{K}^{CSOR})$ and show how to derive the optimal convolution kernel $\omega(t)$. A similar theory can be derived for the discrete-time equivalent of the method.

Finally, the theoretical results are applied to the heat equation and compared against the obtained numerical results. It turns out that $\rho(\mathcal{K}^{CSOR}) \approx 1 - 2\pi h$, where h is the mesh-size of the spatial finite element grid.

[1] M.W. Reichelt, J.K. White, and J. Allen, *Optimal convolution SOR acceleration of waveform relaxation with application to parallel simulation of semiconductor devices*, 1993. (accepted for publication in SIAM J. Sci. Comput.).

PDEX1M – A Softeware Package for the Numerical Solution of Nonlinear Parabolic Systems in One Space Dimension

U. Nowak

A new method for the numerical solution of highly nonlinear, coupled systems of parabolic differential equations in one space dimension is presented. The approach is based on a classical method of lines treatment. Time discretization is done by means of the semi–implicit Euler discretization. Space discretization is done with finite differences on non–uniform grids.

Both basic discretizations are coupled with extrapolation techniques. With respect to time the extrapolation is of variable order whereas just one extrapolation step is done in space. Based on local error estimates for both, the time and the space discretization error, the accuracy of the numerical approximation is controlled and the discretization stepsizes are adapted automatically and simultaneously. Besides the local adaptation of the space grids after each integration step (static regridding), the grid may even move within each integration step (dynamic regridding).

Thus, the whole algorithm has a high degree of adaptivity. Due to this fact, challenging problems from applications can be solved in an efficient and robust way. The algorithm is implemented (FORTRAN 77) in a user friendly software package – PDEX1M. The user of the software can easily set up her/his problem and solve it with the implemented standard method. Alternatively, the user may select special algorithmic variants, e.g. the way how the (optional) moving grid technique is used. Furthermore, the package offers different modes for the linear system solution, Jacobian approximation and solution output generation. Based on tcl/tk there is an easy–to–use graphical user interface available.

Electromagnetic Control for Fluid Flows

S.S. Ravindran

Controlling the fluid flows by internal forcing in electrically conducting flows has wide range of applications such as novel underwater propulsion technologies, fusion reactor technology and nuclear reactors.

In this talk, we consider a velocity field control problem in stationary electrically conducting fluids. Existence and the first order optimality conditions of the optimal control are estabilished. Numerical methods are discussed to solve the State and Adjoint state equations associated with the optimal control problem. Numerical results are presented to show the feasibility of the optimization methods in electromagnetic flow control.

Time–stepping Algorithms for Semidiscretized PDEs based on Rational Approximations with Distinct Real Poles

A.Q.M. Khaliq and D.A. Voss

Time dependent problems in partial differential equations (PDE's) are often solved by the method of lines. In many important instances, the exact solution of the resulting system of ordinary differential equations satisfies recurrence relations involving the matrix exponential function. This function is approximated by a new type of rational function possessing real and distinct poles which, consequently, readily admits a partial fraction expansion thereby allowing the distribution of the work in solving the corresponding linear algebraic systems in essentially backward Euler–like solves on concurrent processors.

Locally one–dimensional splitting methods with enhanced parallelization are developed for multispace problems utilizing Strang–like splitting techniques. The use of rational approximants with distinct real poles in the temporal direction, in collusion with splitting techniques in the spatial directions, creates the potential for efficient coarse grain time–stepping parallel algorithms on MIMD machines. The resulting parallel algorithms possess appropriate stability properties, and are implemented on various parabolic and hyperbolic PDE's from the literature in higher space dimensional problems.

PARALLEL B: PRACTICAL PARALLEL METHODS

PWVODE - a parallel ODE solver based on VODE

K. Burrage and B. Pohl

In this talk a new software package called PWVODE is presented. PWVODE stands for Parallel solver based on Waveform Relaxation using VODE and is intended to work on a wide variety of parallel platforms. Systems of ordinary differential equations are solved in parallel using the waveform relaxation algorithm and allowing the subsystems to overlap. As the integration package for solving the subsystems numerically on each processor, VODE written by Hindmarsh, Brown and Byrne, was chosen.
The package will be introduced and the usage will be explained. Moreover the necessary steps for running your own new problem will be presented. The code will be available via anonymous ftp from both authors.

The Construction of Parallel DIMSIMs for Stiff ODEs and DAEs

P. Chartier

For Runge-Kutta methods, the value of the stability function $R(z)$ in the limit as z tends to infinity as well as the so-called "stiff accuracy" are of great significance for the solution of stiff ODEs and DAEs. The aim of this talk is to discuss the construction of stiffly accurate parallel Diagonally-implicit multi-stage integration methods, known by the acronym DIMSIM, and to compare their performances with other L-stable schemes from the same family.

Time Integration of a 3D Bio-Chemical-Transport Model

B. Sommeijer

The total solution of a three-dimensional model for computing transport of salinity, pollutants, suspended material, etc. together with their bio-chemical interactions in shallow seas, involves many aspects. Each of these has to be treated in an optimal way in order to cope with the tremendous computational task involved. In this contribution we restrict ourselves to the time integration part, paying special attention to properties which make the algorithm suitable for implementation on high-performance architectures. We will discuss an algorithm in which the transport-part (a PDE of convection-diffusion type) and the chemistry-part (in water applications, this is typically a nonstiff ODE) will be treated separately by different integration techniques.

For the transport-part we constructed a special Hopschotch method; for the chemistry-part we considered several explicit Runge-Kutta methods. This algorithm, implemented on a CRAY C90 multi-processor machine (with a clock cycle time of 4.2 nanoseconds), shows a performance of half a gigaflop per processor; moreover, it offers good prospects for parallelization as well. If time allows, aspects like data structures, vectorization of the linear algebra part in the implicit Hopscotch method and of the ODE solver, and numerical aspects of the total method will be discussed.

Step-Parallel Iteration of Implicit ODE Solvers

P.J. van der Houwen

One of the most powerful methods for solving IVPs for ODEs is an implicir Runge–Kutta method such as the Radau IIA methods. These methods are both highly accura te and highly stable. However, the iterative scheme needed for solving the impli cit relations requires a lot of computational effort. The arrival of parallel computer systems have changed the situation in the sense that the effective computationa; effort can be reduced to a large extent. One option is the application of the iteration scheme concurrently at a number of step points on the t-axis. In this talk, the convergence and performance of this approach will be discussed.

PARALLEL C1: HAMILTONIAN PROBLEMS

Conserving Integrators for Nonlinear Hamiltonian Systems with Symmetry

O. Gonzalez

It is shown that conventional time-stepping schemes with supposedly optimal stability properties, such as the Gauss family of implicit Runge-Kutta methods, may exhibit spurious solutions and instability when applied to stiff nonlinear Hamiltonian systems with symmetry. As an alternative, schemes which conserve exactly the Hamiltonian and momentum map are introduced and it is shown that these schemes possess notions of stability analogous to those of the underlying system.

Integration of Nearly Integrable Systems

R. McLachlan

Splitting and composition methods apply particularly well to systems which are close to one which can be solved exactly. Truncation errors at a fixed time can be reduced from $O(1)$ (for a standard method) to $O(\epsilon)$ (for a standard composition method) to $O(\epsilon^2)$ with very little extra computation. In applications to quantum statistical mechanics, even further orders of accuracy in ϵ and Δt can be gained.

PARALLEL C2: GENERAL PROBLEMS

A Dichotomically Stable Integrator for Solving Index-One Differential-Algebraic Equations by Multiple Shooting

R. England

In a number of articles, R.England and R.M.M.Mattheij have considered numerical methods for the solution of stiff boundary-value problems (BVPs) in ordinary differential equations. In the linear case, such a problem may be written as a system of n differential equations

$$\frac{d\mathbf{X}}{dt} = \dot{\mathbf{X}} = \mathbf{L}(t)\mathbf{X} + \mathbf{R}(t) \quad \epsilon\, I\!R^n \qquad (a \le t \le b)$$

subject to n boundary conditions

$$\mathbf{H}_0\mathbf{X}(a) + \mathbf{H}_1\mathbf{X}(b) = \mathbf{C} \quad \epsilon\, I\!R^n.$$

If the problem is well conditioned, then its fundamental modes may be expressed in terms of a dichotomic basis, each member of which has either no significant growth or no significant decay, and in particular the fast modes can be separated into growing modes which are negligible outside a boundary layer near b, and decaying modes, negligible outside a boundary layer near a. Nevertheless, the fast modes control the stability of any numerical method, and much more severely than for stiff initial-value problems, for which there are no fast growing modes. It turns out that a suitable discretization should be dichotomically stable, so that growing modes are represented by growing discrete modes, while decaying modes are represented by decaying discrete modes. The work of England and Mattheij has culminated in a sequential marching algorithm, of multiple-shooting type, for BVPs in ordinary differential equations.

Meanwhile, R.Lamour has developed a multiple-shooting code for fully implicit systems of differential-algebraic equations of index one

$$\mathbf{F}(\dot{\mathbf{X}}, \mathbf{X}, t) = \mathbf{0} \quad \epsilon \, I\!R^n \qquad (a \leq t \leq b)$$

subject to boundary conditions

$$\mathbf{G}(\mathbf{X}(a), \mathbf{X}(b)) = \mathbf{0} \quad \epsilon \, I\!R^n.$$

Using orthogonal projectors $\mathbf{P}, \mathbf{Q}$, he separates the dependent variables $\mathbf{X}(t)$ into "differential variables" $\mathbf{U}(t) = \mathbf{P}(t)\mathbf{X}(t)$, and "algebraic variables" $\mathbf{V}(t) = \mathbf{Q}(t)\mathbf{X}(t)$ whose derivatives do not appear in the problem statement. To avoid a formulation of the multiple-shooting equations which would have a singular Jacobian matrix, he solves the matching equations in $\mathbf{U}_i$, together with the boundary conditions, and the additional equations

$$\mathbf{Q}_0\mathbf{Y}_0 + \mathbf{P}_0\mathbf{V}_0 = \mathbf{0},$$

$$\mathbf{F}(\mathbf{Y}_0, \mathbf{U}_0 + \mathbf{V}_0, t_0) = \mathbf{0},$$

for the variables $\mathbf{Y}_0, \mathbf{V}_0$ which give consistent initial values for $\mathbf{Y} = \mathbf{P}\dot{\mathbf{X}}$ and $\mathbf{V} = \mathbf{Q}\mathbf{X}$ at $t = t_0$. He solves each initial value problem using an integrator based on BDF discretizations, which are clearly not dichotomically stable. It is therefore to be expected that his code may give unsatisfactory results for some stiff two-point BVPs.

This paper describes the adaptation of R.England's dichotomically stable integrator SYMIRK for the solution of systems of differential-algebraic equations of index one, and its implementation into R.Lamour's multiple-shooting code.

New Algorithms for Computing Branches of Secondary Periodic Bifurcation Points

T. F. Fairgrieve

A complete mathematical analysis of the parameterized, autonomous, nonlinear, system of ordinary differential equations $\underline{y}' = \underline{f}\left(\underline{y}; \underline{\alpha}\right)$ requires, in part, a study of the equation's periodic solutions. Software tools for a computational bifurcation analysis of $\underline{y}' = \underline{f}\left(\underline{y}; \underline{\alpha}\right)$ are considered, with a focus on how they compute branches of generic secondary periodic bifurcation points (periodic turning points, period doubling bifurcations and torus bifurcations). There are many bifurcation analysis packages available, however most cannot directly handle the computation of these types of branches. Those that can are slow. For example, when the AUTO package is used to compute branches of periodic turning points in the dimension four coupled Brusselator model, six and a half times more CPU time is required than for computing a generic periodic solution branch in the same model. This ratio grows with the dimension of the system. Furthermore, the Floquet multipliers of these periodic solution bifurcation points are not computed by AUTO, and this can make it difficult to detect subsequent periodic bifurcations.

New algorithms for faster branch computations are derived by considering known properties of the Floquet multipliers of these particular periodic solutions. It is known, for example, that periodic turning points must have an algebraic multiplicity two defective Floquet multiplier at $+1$. This constraint can be used to develop a coupled two-point boundary value problem whose solution is a periodic turning point in the original model. The structure of this boundary value problem is such that it can be solved more quickly than the corresponding system implemented in the AUTO package. Similar constraints and boundary value problems can also be derived for period doubling and torus bifurcation points. The form of the boundary value problems makes it easy to compute the Floquet multipliers along the secondary periodic bifurcation branches, and this assists further bifurcation analysis.

The AUTO package has been modified to include an implementation of these new boundary value problems and algorithms for their solution. Computational results for periodic turning points in the coupled Brusselator model demonstrate a speedup of over two and a half times, and a complexity analysis predicts a speedup factor of up to eight as the dimension of the model increases. In the case of period doubling bifurcation points, the speedup is similar. For torus bifurcation points, a speedup of over four has been observed with the Brusselator problem, and an analysis predicts a speedup of up to eighteen. Further computational studies show that the computed Floquet multipliers converge at theoretically predicted rates, which improves confidence in the numerical results.

Computational Sensitivity Analysis for Parametric Control Problems

H. Maurer

The paper is concerned with the following *parametric nonlinear control* problem $OC(p)$ depending on a parameter p in a Banach space P: Minimize

$$g(x(b),p) + \int_a^b L(x(t),u(t),p)dt$$

subject to

$$\dot{x}(t) = f(x(t),u(t),p)\ ,\ \varphi(x(a),x(b),p) = 0\ ,$$

and mixed control-state constraints

$$C(x(t),u(t),p) \leq 0 \quad \text{for} \quad a \leq t \leq b\ .$$

The functions of appropriate dimensions are assumed to be C^2-functions. The problem $OC(p_0)$ corresponding to a fixed reference parameter $p_0 \in P$ is considered as the unperturbed problem. We shall study stability properties of solutions to $OC(p)$ in a neighborhood of p_0. In [1] – [3] we have developed conditions such that the following stability result holds:

Solution Differentiability : The solution $x(t,p)$, $u(t,p)$ to $OC(p)$ and the associated adjoint variable $\lambda(t,p)$ are C^1-functions with respect to (t,p) for all p in a neighborhood of p_0 and for a.e. $a \leq t \leq b$.

The proof involves three main assumptions: (a) Second-order sufficient conditions [4] are satisfied ; (b) Controllability holds and (c) Junction conditions with the boundary are fulfilled. We shall elaborate on the close relationships between these theoretical conditions and *numerical shooting methods* for solving the underlying boundary value problems.

Solution differentiability is the theoretical basis for performing a numerical sensitivity analysis of the optimal solution with respect to parameters. There is still a deficit of numerical examples illustrating sensitivity analysis. As application we present a detailed numerical study of the Rayleigh problem from electrical engineering. The analysis includes the numerical verification of all stability conditions.

[1] K. Malanowslki and H. Maurer, *Sensitivity Analysis for Parametric Control Problems with Control – State Constraints*, to appear in Computational Optimization and Applications.

[2] H. Maurer and H. J. Pesch, *Solution differentiability for parametric nonlinear control problems*, SIAM Journal on Control and Optimization, 32 (1994).

[3] H. Maurer and H. J. Pesch, *Solution differentiability for parametric nonlinear control problems with mixed control-state constraints*, Control and Cybernetics, 23 , pp. 201-227 (1994).

[4] H. Maurer and S. Pickenhain, *Second – Order Sufficient Conditions for Control Problems with Mixed Control – State Constraints*, to appear in J. of Optimization Theory and Applications.

The DAE-Index in TCAD-Based Electric Circuit Simulation

M. Günther and U. Feldmann

Numerical simulation in the time domain is an important tool in the design of electric circuits nowadays. As well time as money is saved by testing and optimizing circuits without building prototypes. The network equations of highly integrated circuits with thousands of elements cannot be derived analytically. Commercial TCAD-based simulation packages are based on the scheme of Modified Nodal Analysis to generate the equations automatically. This approach involves a redundant set of variables and that leads to differential-algebraic equations (DAE's).

The structure of the DAE-system and its index depend mainly on the applied modeling technique for the circuit elements. Two main types of network equations have to be distinguished: the *capacitance-oriented* and *charge-oriented* formulation. The classical capacitance-oriented approach is based on node potentials and currents only. One gets systems of quasilinear-implicit form: The dynamics is described by the capacitance matrix which is in general very sparse and asymmetrical.

In the charge-oriented approach charges are introduced as additional state variables to describe the dynamic charge flow in integrated MOS-circuits. This yields systems of linear-implicit form: The network topology is reflected by the incidence matrix. The charges are defined explicitly as a function of the node potentials.

We will show how this approach can be used to assure charge conservation independently of the particular charge equations, and that it is favourable to reduce errors of numerical integration as well.

Additionally, the index and the structure of the network equations depend on the mathematical model in different ways: Basic network elements such as capacitances may be described by linear or nonlinear models. Depending on the desired accuracy transistor models with increasing complexity of circuit structure for modelling parasitic elements are used in practical applications. Partially their special structure may lead to e. g. loops of capacitors and voltage sources, thus increasing the index of the DAE-system. We will show how to regularize such models.

Efficient Steady-State Analysis of Mildly Nonlinear Electronic Circuits

P. Feldmann and R. C. Melville

Designers of communications circuitry – both at baseband and radio frequencies – are concerned with simulation questions (harmonic distorsion, intermodulation, compression point, etc.) which all come under the heading of "mildly non-linear" phenomena.

The method of *Harmonic Balance* ([1],[2]) is well-established as a simulation technique for nonlinear circuits driven by one or more periodic inputs. A particular advantage of the harmonic balance method is the ease with which it handles the "two tone" case of intermodulation distortion. The gist of the method is to write each waveform in the circuit as a Fourier series truncated to N coefficients, then replace the circuit's differential equations by a system of non-linear, algebraic equations involving the Fourier coefficients. This is possible because the derivative with respect to time of a Fourier series is just an algebraic operation. A numerical technique, such as Newton's method, is then employed to solve the resulting system of non-linear equations.

However, the system of equations can become rather large, since *each* waveform is replaced by a vector of N complex coefficients; N can be on the order of 128 for a two-tone study. A circuit with, say 1000 waveforms, would then generate a total system of 128000 equations in 128000 unknowns. Most numerical methods for solving larger systems of equations require the *Jacobian Matrix* of the equations to be formed at each step of an iterative process. In the case of harmonic balance equations, this matrix is rather dense, therefore, forming and factoring this matrix becomes a computational bottleneck for even medium-sized circuits (say, 50 transistors).

In this paper, we describe an implementation of a harmonic balance tool which circumvents the computational bottleneck associated with this large Jacobian matrix by using an *iterative linear solver* which only requires multiplication of a vector by the Jacobian matrix or its transpose. We show that the time to multiply the Jacobian matrix with a vector grows only slightly faster than linearly with the total number of unknowns. A pre-conditioner for the iterative linear solver is proposed which facilitates rapid convergence of the iterative method, provided that the circuit is operating in the mildly non-linear regime as mentioned above. Our implementation enables the simulation of circuits much larger than can be handled with other implementations of harmonic balance. However, strongly non-linear behavior cannot be analyzed with the current tool.

Our method is based on two novel results. The first, is the decomposition of the large and dense Jacobian matrix of the harmonic balance system of equations into a number of relatively inexpensive-to-apply linear operators. This decomposition makes possible the solution of very large problems through the use of iterative linear solvers which avoid the storage and factorization of the Jacobian matrix. However, iterative linear solvers converge reliably only if a good preconditioner is available. The second contribution of this paper is the use of the linearized circuit Jacobian matrix as preconditioner. This preconditioner is based on solid engineering intuition, is adequate for all circuits operating in a mildly nonlinear regime, and is inexpensive to apply. Tensor notation provides a compact and elegant way to manipulate the structured matrices arising in the analysis.

[1] K. S. Kundert, J. K. White and A. Sangiovanni-Vincentelli, *Steady-state Methods for Simulating Analog and Microwave Circuits*, Kluwer, Boston, MA., 1990.

[2] R. J. Gilmore and M.B. Steer, *Nonlinear circuit analysis using the method of harmonic balance - a review of the art*, Int. J. on Microwave and Millimeter Wave Computer Aided Engineering, Vol. 1, Jan. 1991.

Dynamic Optimization Algorithms for Process Engineering

L. T. Biegler, J. Albuquerque and P. Tanartkit

Dynamic process systems have special characteristics that need to be considered for optimization. While they often consist of large, nonlinear models, they frequently have relatively few degrees of freedom. Moreover, while many "open loop" systems are characterized by stable dynamic modes, systems with unstable modes can occur in process control applications, as well as reactor models. These systems are usually modeled as differential-algebraic equations (DAEs) and active state variable constraints can induce high

index solution profiles for at least part of the time domain. Finally, the right hand sides of these DAEs can be highly nonlinear and are frequently represented by calculation procedures which can make higher derivative information difficult to obtain.

To formulate an optimization strategy for these systems, we first concentrate on BVP formulations whereby the DAE system is discretized using collocation on finite elements. Here we rely on adaptations of existing results and codes (e.g, COLDAE by Ascher and Spiteri, 1993) to carry out the discretization and solution. To address the solution of the nonlinear programming problem, we develop a reduced Hessian Successive Quadratic Programming (rSQP) strategy that exploits the structure of the collocation solver. By partitioning the variables to lie within range and null spaces of the normals of the collocation equations, second derivative information need only be constructed or approximated in the null space. Thus, "nullspace" steps are determined by an efficient dual quadratic programming solver while "rangespace" steps are obtained from the collocation equations themselves. In this approach, we partition the these spaces so that only "Newton" steps are required from the collocation solver (e.g., COLDAE) and, as a result, Lagrange multipliers for the collocation equations are not calculated (nor required) for the SQP algorithm. As a result, the combined approach is relatively easy to implement and still leads to an efficient optimization strategy for problems with few degrees of freedom.

An alternate strategy has also been implemented that handles problems with many degrees of freedom more effectively. This simple approach repeatedly applies efficient linear BVP solvers to the optimality conditions. However, this approach requires full Hessian information (or its approximation) as well as a more "open" formulation of the collocation equations, without benefit of existing solvers and procedures.

Either approach can also be extended in a number of ways to further address dynamic optimization problems. First, the placement of finite elements to ensure accurate approximations has been explored in a two-level optimization strategy. A fixed element problem is solved in an inner level, while placement and optimization of the elements occurs at the outermost level. While this approach seems clumsier than a simultaneous strategy, it leads to a much more reliable approach. Moreover, the above SQP strategies can also be applied to unstable initial value problems, which can be stabilized by detecting and incorporating dummy boundary conditions in the optimization strategy. Preliminary analysis and evaluation of these this approach will be discussed. Large-scale implementation of these approaches is also currently the focus of this research.

Finally, these concepts will be demonstrated on a number of process optimization problems including solution of optimal profiles for nonisothermal reactors, optimal design of catalyst pellets and on-line reconciliation of process data. These will illustrate the characteristics mentioned above including problems unstable modes and problems with few to many degrees of freedom.

PARALLEL D1: HIGH QUALITY COMPUTATION USING FAST AUTOMATIC DIFFERENTIATION

High Quality Computation Using Fast Automatic Differentiation

K. Kubota

Recently, we can perform the arbitrary (finite) precision arithmetics with the help of symbolic and numerical manipulators, some libraries, etc. Thus, we can easily estimate accumulated rounding errors generated

in the numerical computation using floating-point numbers, thereby, we can compute improved or partially corrected results with the estimations. But it may be required that an investigation on the rounding errors in the improved results themselves so as to make the second improved results. Moreover, another investigation on the second improved results might be needed. After all, even if we use the arbitrary (finite) precision arithmetics, we must consider on rounding errors in partially corrected results from a standpoint where we know the only bounds of the absolute values of the rounding errors and we never know its values nor signs.

A method for estimating the accumulated rounding errors are practically realized by means of a technique called fast automatic differentiation, or reverse mode automatic differentiation. It can inexpensively compute all the partial derivatives with respect to all the intermediate results. The partial derivatives are essential entities in the well-known recurrence formula for estimating accumulated rounding errors. Furthermore, combining the fast automatic differentiation and the interval computation, we can compute their rigorous upper bound [1].

The similar situation appears in the initial value problem in ODE. There are many elaborate techniques to improve the numerical solutions, however, we consider the global error from the same standpoint. That is, we know the bound of the local truncation error but do not their values nor sings. Regarding the recurrence formula as the adjoint equation of ODE, we will point out the analogy between the estimation of accumulated rounding error and the estimation of global error in ODE from the viewpoint of high quality computation.

[1] K. Kubota and M. Iri, *Estimates of rounding errors with fast automatic differentiation and interval analysis*, J. of Information Processing, vol. 14, pp. 508–515, 1991.

PARALLEL D2: DELAY AND VOLTERRA EQUATIONS

Application of Adjoint Equations in Mathematical Modelling of Infectious Diseases

G.A. Bocharov

Quantitative prediction and control of the dynamics of infectious diseases in a host imply an application of mathematical models of increasing resolution. The examples of multiparameter nonlinear delay models used for parameter estimation of hepatitis B and influenza are given by [2,3]. An important problem is to predict the changes in disease dynamics under the influence of various factors, and sensitivity analysis is a basic tool to investigate the predictions of numerical models. Closely related is the inverse problem of determining the deviations in the immunity parameters underlying observed variations of the infection course. Efficient technique to accurately estimate the gradient of an objective function is a key element of the parameter estimation procedures [4].

Adjoint methods are applied for studying the sensitivity of objective functions, depending on model solution, to deviations of the parameters of the problem from "norms", within the framework of the perturbation theory [1]. For an operator, representing the main system of delay-differential equations, the adjoint one is introduced on the base of the Lagrange relation. The adjoint systems of equations are derived for a

simple mathematical model of infectious disease and the mathematical model of antiviral immune response. The solution to the adjoint problem depends on a forcing term determined by the objective function being studied.

Numerical issues of the sensitivity calculations are presented. Computational techniques for the integration of direct and adjoint system of equations with a given accuracy are based on the modification for constant delay systems [4] of the Gear's implementation of BDFs. The Nordsieck vector provides a 'built-in' continuous interpolant for approximating with a given accuracy the right-hand side function of the adjoint system. The efficiency of an adjoint approach is compared with respect to the direct sensitivity analysis, in terms of the computing time and accuracy, for the mathematical model of influenza.

Joint work with G. I. Marchuk.

[1] G.I. Marchuk, *Adjoint equations and analysis of complex systems*, Kluwer Publishing House, 1995, in press.

[2] G.I. Marchuk, A.A. Romanyukha, G.A. Bocharov, *Mathematical model of antiviral immune response. II. Parameter Identification for Acute Viral Hepatitis B*, J. theor. Biol., 151 (1991) pp. 41–70, 1991

[3] G.A. Bocharov and A.A. Romanyukha , *Mathematical model of antiviral immune response. III. Influenza A Virus Infection*, J. theor. Biol. 167, pp. 323–360, 1994

[4] Bocharov G.A. and Romanyukha A.A. Numerical treatment of the parameter identification problem for delay-differential systems arising in immune response modelling. Appl. Numer. Math. 15, pp. 307–326, 1994

Stability Properties of Natural Runge-Kutta Methods for Delay–Differential–Algebraic Equations

T. Koto

A natural Runge-Kutta (RK) method is a RK method which has a special continuous extension; it is equivalent to a projection method in some polynomial space, and a RK method derived from collocation, e.g., the Gauss method is a typical instance of such methods. Although they are generally treated as numerical methods for delay differential equations (DDEs), they can be also applied to delay-differential-algebraic equations (DDAEs) directly if their Runge-Kutta matrices are invertible. We examine the stability properties of natural RK methods for DDAEs using linear DDAEs as test equations. More specifically, we consider the initial value problems in DDAEs of the form

$$\begin{aligned} \frac{dx}{dt} &= L_{11}x(t) + L_{12}y(t) + M_{11}x(t-\tau) + M_{12}y(t-\tau), \\ 0 &= L_{21}x(t) + L_{22}y(t) + M_{21}x(t-\tau) + M_{22}y(t-\tau), \end{aligned}$$

and apply a natural RK method under the condition that L_{22} is invertible. Here, $\tau(>0)$ is a constant delay and L_{ij}, M_{ij} denote constant matrices. Differentiating the latter equation, we obtain a neutral DDE. We can thus derive, by a standard technique, a condition for the solution $x(t)$, $y(t)$ to disappear as $t \to \infty$ for any τ and any initial function. Under this condition we can show the following results: if the natural RK method is A-stable, then the numerical solution never diverges for any constant stepsize of the form $h = \tau/k$, where k is a positive integer; moreover, if the method is A-stable and its stability function, say $r(z)$, satisfies $\mid r(\infty) \mid < 1$, then the numerical solution converges to zero whenever the stepsize takes the

same form as above.

The same results hold also, e.g., for DDAEs of the form

$$\begin{aligned} \frac{dx}{dt} &= L_{11}x(t) + L_{12}y(t) + M_{11}x(t-\tau) + M_{12}y(t-\tau), \\ 0 &= L_{21}x(t) \qquad\qquad + M_{21}x(t-\tau), \end{aligned}$$

where $L_{21}L_{12}$ is invertible. This test equation corresponds to index-two DDAEs of the Hessenberg form.

A Numerical Method Based on a Continuous Runge-Kutta Formula for Delay Differential Equations

H. Hayashi and W. Enright

An approach for the numerical solution of the initial value problems for delay differential equations (DDEs) will be explained. The underlying idea (which is a standard approach) is to adapt an initial value problem solver for ordinary differential equations (ODEs) without delay. We have adapted a continuous Runge-Kutta method with defect based error control. There are three major numerical difficulties to be considered: the solution must be evaluated somewhere other than mesh points; discontinuities may occur in various orders of the derivative of the solution; the delay argument may fall in the current step or may even vanish. The first difficulty is easily resolved by using a continuous method. For the second difficulty, we have adopted the 'automatic' technique for handling discontinuities for ODEs by Enright et al. The idea is to monitor the size of the defect on each step and to detect and locate (using a bisection scheme) when and where a discontinuity is encountered. For the last difficulty, we have used an iterative scheme with an initial approximation determined by an extrapolation or by a special interpolant. In most of steps the extrapolation is used since the order of the error is usually higher than that by using the special interpolant. The special interpolant is only used in the first step of integration and on steps right after discontinuities. In such steps the extrapolation is not available or reliable.

Note that our approach results in a variable stepsize method which can be applied to problems with state dependent delays. It can also be applied to any continuous Runge-Kutta formula and such formulas up to order 8 have been widely investigated. We will restrict our attention to an order 6 method. We will quote some convergence results and also show that our method solves DDEs effectively relative to other existing methods (which are all based on Runge-Kutta formulas) by presenting summaries of numerical testing. Furthermore, the extension of our approach to neutral delay differential equations will be discussed.

On the Discretization of Volterra Integral Equations with Variable Delay

H. Brunner

Let $S_{m-1}^{(-1)}(\Pi_N)$ denote the space of (real) piecewise polynomials of degree at most $m-1$ ($m \geq 1$), and let $u \in S_{m-1}^{(-1)}(\Pi_N)$ be the collocation solution approximating the solution of either a classical Volterra integral equation of the second kind or of a second-kind Volterra integral equation with *constant delay*. Denote by u_{it} the corresponding iterated collocation solution.

If these integral equations are obtained, respectively, from the ODE

$$y'(t) = ay(t) \qquad (t \geq 0),$$

and the DDE

$$y'(t) = ay(t) + by(t-\tau) \qquad (t \geq 0),$$

where a and b are constants, $\tau > 0$, and if v_n is the approximation generated by the implicit RK method based on the collocation parameters used in the computation of u, then it is well known that

$$u_{it}(t_n) = v_n \qquad (n = 1, \ldots, N).$$

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

$$y'(t) = ay(t) + by(qt), \qquad y(0) = y_0, \tag{0.12}$$

and

$$y(t) = y_0 + \int_0^t ay(s)\, ds + \int_0^{qt} \frac{b}{q}\, y(s)\, ds\,. \tag{0.13}$$

In other words, the dynamics of certain (collocation) discretizations of (1) (which has been studied extensively in recent work by Buhmann and Iserles) is not identical with that of analogous discretizations of the integral equation (2). On the other hand, we will also show that, in spite of this difference, collocation and iterated collocation using the Gauss points lead to local superconvergence of order $p = 2m$ on the mesh Π_N for both (1) and (2) (and their more general linear versions).

Continuous Collocation Approximations of Solutions of First Kind Volterra Equations

J.-P. Kauthen and H. Brunner

We consider the first kind Volterra integral equation

$$\int_0^t K(t,s)y(s)\, ds = g(t), \qquad t \in I = [0,T],$$

where g and K are supposed to be sufficiently smooth functions on their respective domains and satisfying $g(0) = 0$ and $|K(t,t)| \geq \varrho > 0$ for all $t \in I$.

We are interested in continuous polynomial spline collocation approximations of y. For this purpose we consider the subdivision Π_N of the interval $I = [0,T]$ defined by $t_n = nh$ where the (constant) stepsize is given by $h = T/N$ $(N > 0)$. Let $0 < c_1 < c_2 < \ldots < c_m \leq 1$ $(m \geq 1)$ be the collocation parameters and $t_{nj} = t_n + c_j h$, $j = 1, \ldots, m$, $n = 0, \ldots, N-1$, the collocation points. We seek an approximation u of y in the polynomial spline space

$$S_m^{(0)}(\Pi_N) = \{u \in C(I) : u_n = u|_{[t_n, t_{n+1}]} \in \pi_m\}.$$

This approximation satisfies the collocation equation

$$\int_0^{t_{nj}} K(t_{nj}, s)u(s)\, ds = g(t_{nj}), \qquad j = 1, \ldots, m,\ n = 0, \ldots, N-1,$$

the continuity conditions $u_{n-1}(t_n) = u_n(t_n)$, $n = 1, \ldots, N-1$, with initial value $u(0) = y(0) = g'(0)/K(0,0)$.

It is known [1] that if $c_m = 1$, the collocation error $e = y - u$ behaves like $\|e\|_\infty = \mathcal{O}(h^{m+1})$, as $h \to 0$ with $Nh = T$ for all $m \geq 1$ if, and only if, the collocation parameters c_i verify $\prod_{i=1}^{m-1}(1 - c_i)/c_i < 1$, whereas the case $c_m < 1$ remained an open problem. We now filled this gap. Necessary and sufficient conditions for

convergence for the case $c_m < 1$ are given. The results are based on properties of Runge-Kutta collocation methods characterized by $c_1 < c_2 < \ldots < c_m$ and the additional parameter $c_0 = 0$. It follows in particular that if the collocation parameters are symmetrical, i.e. if $c_i = 1 - c_{m+1-i}$, $i = 1, \ldots, m$, then the collocation approximation u does not converge to the solution y. Moreover if $m = 1$ there does not exist a convergent collocation method in $S_1^{(0)}(\Pi_N)$.

[1] H. Brunner and P.J. van der Houwen, *The Numerical Solution of Volterra Equations*, North-Holland, Amsterdam, 1986.

Friday AM

PLENARY SESSION

A Critique of the Symmetric Multistep Methods

A. Toomre and G. D. Quinlan

Used with care, the high-order "symmetric multistep" methods proposed by Quinlan and Tremaine (1990, Astron.J., 100, 1694) for the long-term numerical integration of planetary orbits in our solar system offer impressive gains in accuracy or efficiency over classical methods like Adams or Stormer. But these fast new methods are fraught with interesting perils of their own, all stemming from the undamped free or "parasitic" oscillations admitted by their difference equations. As we will illustrate, such jitters can lead to quite a few spurious resonances and even to some Mathieu-like instabilities for test problems as humble as a single Kepler ellipse or the hard-spring oscillator $x'' = -x^3$. In the first 2/3 or so of this talk, Toomre will describe the main pros and cons of these methods, whereas in the last 1/3 Quinlan will discuss to what extent their oscillations can be avoided or minimized in practice.

On BDF for Stiff Problems in ODEs, DAEs, PDEs, and BIEs

C. Lubich

This talk is about recent convergence results for BDF methods applied to a variety of "stiff" problem classes. These include ordinary differential equations of singular perturbation type, differential-algebraic equations describing the motion of strongly damped mechanical systems, reaction-diffusion equations with slow and fast chemistry, and quasilinear parabolic partial differential equations. The techniques used in the theoretical analysis have also led to the discovery of a promising class of BDF-based time discretization methods for time-dependent integral equations. This is illustrated for the single-layer potential boundary integral equations of the heat and (strongly or otherwise) damped wave equations.

PARALLEL A: INITIAL VALUE ODEs

Component Based Modelling

P.G. Thomsen

A modelling system based upon components as building blocks in a network is presented. The basic equations are derived from conservation principles in the nodes of the network. They form a system of DAE's. The components will in general be nonlinear with possible state changes. Systems are accepted in both explicit and implicit form. The approach to defining building blocks is object oriented based upon three component classes one for the system component one for the network links and one for the states of the component.

The system consists of a formal language, an interpreter and the interface to the object library of GODESS. The modelling language and the interpreter allows for algebraic manipulations like differentiation. The analytic Jacobean may be derived automatically.

GODESS is a Generic ODE Solving System implementing an Object Oriented platform for solving systems of ODE's and DAE's. The choice of method is made by the user who can define his own one-step method and our default choice is a GERK method derived by A. Kværnø.

Equilibrium States of Adams Codes

G. Hall

The purpose is to analyse the performance of variable-step Adams codes on mildly stiff problems. For the general case, where the dominant eigenvalue of the Jacobian is complex, algorithmic steady states are defined using a constant stepsize corresponding to the boundary of the stability region. By considering perturbations about the steady state it is possible to predict the behaviour of the algorithm with respect to different stepsize strategies.

Limiting Formulas of Eight-Stage Explicit Runge–Kutta Method of Order Seven

H. Ono

It is well known that eight-stage explicit Runge-Kutta formulas are of order six. While by taking the limit as the first abscissa approaches zero, the formulas can achieve seventh order. Such formulas are called limiting formulas. In which the evaluations of the second derivatives are required. In this paper, eight-stage seventh order limiting formulas using the second derivatives are derived. And based on these limiting formulas, new eight-stage numerically seventh order methods without derivatives are proposed.

Runge-Kutta Magic or Is There an Easy Way for Obtaining the Order Conditions of Runge-Kutta Methods ?

S.N. Papakostas

The estimation of the order conditions for Runge-Kutta methods (and much more the construction of efficient methods) has always been considered as a difficult and complicated subject. Our current understanding in this area stems from the works of many people, most notably those of Kutta, Nystrom, Gill, MERSON, Butcher, Shanks, Rosen, Hairer, ... In this talk we shall present a new alternative approach, where no graphical objects are necessary for realizing order conditions, we will explain how one manually (or even automatically) can compute them and what is the most important, how the practical search for finding efficient methods may be benefited by this new approach.

It is the hope of the present speaker that he will be able to persuade his audience that no more than 30′ of thinking is necessary for one person to become acquainted with the order conditions for Runge-Kutta methods, to understand what they are and why they are those they are. We will also present how other integration methods may be studied in a similar way and how a general rule of simplifying assumptions may be embodied directly into the way of our perception of such methods.

This talk is a compilation for this conference of a more general work on the subject of order conditions for integration methods for ODE's, where we present a more rigorous mathematical development. Here instead, we shall try to explain intuitively and heuristically a reasonable amount of motivations for a more general theory.

Automating the Construction of Runge-Kutta Methods by Computer

M. Sofroniou

Runge-Kutta methods find wide-scale application in the numerical solution of certain types of ordinary differential equations. The derivation of these methods is a very challenging mathematical problem with a long historical background. A state-of-the-art tool for the numerical analysis of ordinary differential equations is described. This considerably lightens the task of the derivation and subsequent analysis of Runge-Kutta methods.

The first difficulty in deriving Runge-Kutta methods is in establishing the order conditions, which help to ensure that the numerical solution closely models the underlying physical system. The second difficulty is in obtaining solutions: the equations are nonlinear in the coefficients and exhibit combinatorial explosion in the number of constraints as the order is increased. The work described here concerns the automation of the derivation process using computer algebra and indicates how solutions may be obtained. The package will be included for distribution in the next major release of Mathematica.

Topics which will be discussed include:

1. Trees and elementary differentials. The representation and construction will be discussed.
2. Order conditions and classes of methods distinguished. Both tensor and index notations are provided.

3. Controlling non-linearity - Butcher's simplifying assumptions. The default behaviour is outlined along with examples of how to construct alternative assumptions.
4. Overview, examples and discussion of a solution process.
5. Computer based proofs. This includes the resolution of a long-standing conjecture that no computer algebra system can establish the non-existence of 5 stage 5th order explicit Runge-Kutta methods.
6. Application to open research problems. Extensions to the package are outlined, illustrating how new methods can be constructed. In particular emphasis will be focused on building a formalism for symplectic Runge-Kutta methods and the investigation of Runge-Kutta methods for quadratic ODEs.

A Numerical Modelling of the Aerosol Formation Kinetics

A.I. Levykin

Two numerical algorithms for solving the Smolouchovsky system of coagulation equations:

$$\frac{dN_1}{dt} = -N_1 \sum_{i=1}^{\infty} \beta_{1i} N_i + \sum_{i=2}^{\infty} E_i(1+\delta_{2i}) N_i - W_1 N_1 + F(t),$$

$$\frac{dN_l}{dt} = \frac{1}{2} \sum_{i+j=l} \beta_{ij} N_i N_j - N_l \sum_{i=1}^{\infty} \beta_{li} N_i + E_{l+1} N_{l+1} - E_l N_l - W_l, \; l \geq 2,$$

governing the kinetics of aerosol formation with account of source, depletion of l-mers due to monomer evaporation and to well deposition are reported.

The first algorithm is based on the approximation of solution by δ-functions, linear functions and B-splines. The system ODE of derived is solved by the explicit Runge-Kutta scheme using the automatic control of accuracy and of stability. In the second algorithm we used a grid-adapted to the solution. The resulting implicit ODE was solved by (m,k)-Rosenbrock type method, using approximation matrices of derivatives. A comparison of some characteristics of the solution calculated by two methods suggested with experiments of photolysis of iodinebensene-ozone mixture.

PARALLEL B: LINEAR ALGEBRA

Large stiff systems require the solution of linear and nonlinear systems. In this minisymposium, iterative solver issues are addressed.

Preconditioned Krylov Methods in Tokamak Edge Plasma Modeling

P. Brown and A. Hindmarsh

Incomplete factorization techniques are used as preconditioners in an iterative solution of the linear systems arising in the solution of time-dependent and time-independent Tokamak edge plasma models. After discretizing in space, the resulting models can be either ordinary differential equations or differential algebraic systems, depending on the particular problem of interest. Various reordering strategies are used to reduce fill-in and improve the overall effectiveness of the techniques.

Preconditioned Krylov Methods for Computing Spacetime Curvature

S. Lee

The equations that govern the behavior of physical systems can often be numerically solved via a method of lines (MOL) discretization and differential-algebraic equation (DAE) solvers. For example, the behavior of black holes can be modeled by treating the Einstein equations of general relativity as an index-2 DAE. To efficiently compute the evolution, large nonsymmetric linear systems must be solved at each time step. In this context, we have found that a certain symmetric (and possibly indefinite) preconditioner is often effective.

The implementation of this preconditioner, and the important properties of the preconditioned matrices are discussed. We also report the effectiveness of using the preconditioner and Krylov methods in computing the spacetime curvature that black holes generate.

QMRPACK and Applications

N. Nachtigal and R. W. Freund

QMRPACK is a FORTRAN-77 software package implementing various linear systems solvers based on the QMR algorithm, as well as an eigenvalue code based on the look-ahead Lanczos algorithm. This talk will review the algorithms covered and discuss their implementation in QMRPACK. We will also present numerical examples that illustrate the capabilities of the package.

Robust Preconditioning Techniques for General Sparse Linear Systems

Y. Saad

The numerical solution of linear systems arising from fluid flow problems and other applications can be rather challenging for iterative methods. In this talk we compare a number of standard preconditioning approaches to solve these problems. We test two accelerators, GMRES and DQGMRES, combined with a few threshold based preconditioners such as ILUT and approximate inverse techniques, on a number of linear systems arising from various models.

PARALLEL C1: PARALLEL METHODS FOR ODEs

DIMSEMs — Diagonally IMplicit Single-Eigenvalue Methods for the Numerical Solution of Stiff ODEs on Parallel Computers[2]

R. Enenkel and K. Jackson

We describe two new classes of General Linear Methods (GLMs) suitable for solving stiff ordinary differential equations on parallel computers. A GLM for the scalar initial-value problem

$$\begin{aligned} y'(x) &= f(y(x)), \quad x \in [x_0, x_e], \\ y(x_0) &= y_0, \end{aligned} \tag{0.14}$$

has the form

$$\begin{aligned} Y_n &= A_1 y_n + hB_1 F(Y_n) \in \mathbb{R}^s, \\ y_{n+1} &= A_2 y_n + hB_2 F(Y_n) \in \mathbb{R}^r, \end{aligned} \tag{0.15}$$

where h is the stepsize, $F(Y_n)$ is the vector formed by applying f to each component of Y_n, $A_1 \in \mathbb{R}^{s\times r}$, $B_1 \in \mathbb{R}^{s\times s}$, $A_2 \in \mathbb{R}^{r\times r}$ and $B_2 \in \mathbb{R}^{r\times s}$ are matrices of coefficients which determine the method. The components of the external stages y_n may, in different methods, represent approximations to the solution at various points, derivatives of the solution, or other quantities from which the solution may be recovered. Although we have described the GLM (0.15) for the scalar problem (0.14), all our results extend to systems of equations in the usual way.

We will discuss how to find implicit GLMs with the following properties.

1. B_1 is diagonal. Thus the linear system which arises when Y_n is computed by Newton's method decouples, allowing for an efficient parallel implementation.
2. The stability matrix has no spurious eigenvalues. That is, only one eigenvalue of the stability matrix is non-zero. (This property distinguishes our methods from Butcher's DIMSIMs, which share property 1.)

[2]This work was supported in part by the Natural Sciences and Engineering Research Council of Canada and the Information Technology Research Centre of Ontario.

3. The methods have order and stage order $r-1$, with $s = r-1$ or $s = r$. The high stage order permits the methods to retain their order on problems where order reduction might otherwise be a problem.
4. The methods are L-stable, making them suitable for the solution of stiff problems.

We have developed a class of methods of any order satisfying conditions 1–3, with $s = r-1$, from which L-stable methods of orders 2–6 were found and tested. In addition, a class of methods of any order satisfying properties 1, 3 and 4, with $s = r$, was constructed and methods of orders 2–6 derived and tested.

The talk will present some theorems bounding the order of DIMSEMs, and describe the methodology used to derive our schemes. We have so far performed only fixed-stepsize numerical testing, but, by the time of the conference, we expect to have completed testing variable-stepsize implementations and possibly performed some performance measurements on a parallel machine as well.

Parallel SIRK-Based Methods

B. Orel

Runge-Kutta methods are widely used in the numerical treatment of stiff ODEs. We will discuss the construction of a class of multi-implicit RK methods, based on multiply p-restricted Pad'e approximations to the exponential function. These methods are intenteded for use on parallel computers.

The constructed RK method for solving wide range of problems from stiff and singularly perturbed ODEs to DAEs on parallel computers will have the following properties:

- an reliable estimate of the local error is available at each step;
- the method is L-stable;
- the method is stiffly accurate;
- the eigenvalues of the coefficients matrix are real and distinct.

Embedded pairs of RK methods of order 3(2) with 4 stages, of order 4(3) with 5 stages and order 5(4) with 7 stages will be presented.

A Generalization of Certain Classes of Parallel Block Methods for Second Order IVP's

S. O. Fatunla and M. N. O. Ikhile

This paper provides a conceptual framework for the generalization of some parallel Block Methods (BM) including Fatunla[1991, 1994a, b] for the second order Initial Value Problems (IVP's) $y'' = f(x, y)$, $y(a)$, $y'(a)$ given. The order conditions of these methods are also discussed whose relative advantages of these schemes include the anticipated speedup, adequate stability at the origin and cheap error estimators. The scheme is extended to parallel BM for massively parallel systems.

Two–Step Runge–Kutta Methods for Ordinary Differential Equations

Z. Jackiewicz

A general class of two–step Runge–Kutta methods is studied, which depend on stage values at two consecutive steps. These methods are special cases of general linear methods introduced by Butcher and are quite efficient with respect to the number of function evaluations. General order conditions are derived using the approach proposed recently by Albrecht, and examples of methods are given up to the order five. These methods can be divided into four classes which are appropriate for the numerical solution of nonstiff or stiff differential systems in sequential or parallel computing environments. High order and high stage order are preserved on nonuniform meshes with large variations in ratios between consecutive stepsizes.

This is a joint work with S. Tracogna.

PARALLEL C2: BOUNDARY VALUE METHODS FOR INITIAL–VALUE ODEs

Symplectic Boundary Value Methods for Hamiltonian Systems of Ordinary Differential Equations

L. Brugnano

In the last few years many efforts have been made in the study and definition of symplectic numerical methods for Hamiltonian systems of Ordinary Differential Equations. Even if symplectic integrators have been found in the class of Runge-Kutta methods and in the class of One-Leg methods, there are no good integrators in the class of Linear Multistep Formulae. This is essentially due to the fact that the symmetry property [3] required by LMF to be symplectic weaken their usual stability properties. This barrier may be overcome by considering the use of LMF as Boundary Value Methods (BVMs). This approach consists in the approximation of a given continuous initial value problem by means of a suitable discrete boundary value one. These methods have been studied succesfully and generalized definitions of 0-stability and Absolute stability have been recently given [1,2]. By using this approach, it is possible to define virtually infinite families of symplectic BVMs. In particular, we shall describe only three of such families of methods which provide symplectic methods of arbitrary high order. Moreover, the stability properties of these methods are excellent. In fact, for all of them the region of Absolute stability (in the BVM sense) coincides with the left half of the complex plane. Finally, since all these methods are symmetric, they have been found very effective also in the approximation of continuous boundary value problems [1].

[1] L. Brugnano, D. Trigiante, *High Order Multistep Methods for Boundary Value Problems, Proceedings of NUMDIFF-7 (Appl. Numer. Math., to appear).*
[2] L. Brugnano, D. Trigiante, *Solving ODE by Linear Multistep Formulae: Initial and Boundary Value Methods*, (in preparation).
[3] T. Eirola, J.M. Sanz-Serna. *Conservation of Integrals and Symplectic Structure in the Integration of Differential Equations by Multistep Methods, Numer. Math.* 61 (1992) 281–290.

Boundary Value Methods for Nonlinear ODEs: Unique Solvability and Stability Properties

F. Iavernaro

Considerable attention has been always devoted to the development of accurate methods with good stability properties for the solution of initial value ODEs:

$$\begin{cases} \mathbf{y}' = \mathbf{f}(t, \mathbf{y}) & t \in [t_0, t_f] \\ \mathbf{y}(t_0) = \mathbf{y}_0. \end{cases} \tag{0.16}$$

In general an improvement of stability of high order methods implies a remarkable increase of computational complexity. A possible way to overcome this problem is to find methods which can be efficiently implemented on a parallel computer.
Boundary Value Methods (BVMs) fulfill both the requests:

- interesting stability properties associated to arbitrary order of convergence;
- efficient parallel implementations.

These methods tackle the numerical solution of (0.16) in a completely different way than the classical approaches. The initial value problem (0.16) is considered as a two-point boundary value problem with a given value at the left endpoint. The numerical solution is given simultaneously on the grid points by solving a system of equations. As a consequence it is possible to control the global error rather than the local one.
A k-step BVM with m initial and $k-m$ final condition takes the form:

$$\begin{cases} \displaystyle\sum_{i=0}^{k} \alpha_i \mathbf{y}_{n-m+i} = h \sum_{i=0}^{k} \beta_i \mathbf{f}_{n-m+i}, & n = m, \ldots, N, \\ \mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{m-1}, \mathbf{y}_{N+1}, \ldots, \mathbf{y}_{N+k-m} & \textit{given} \end{cases} \tag{0.17}$$

where h is the stepsize and α_i and β_i are chosen so that (0.17) has a given order. If $m = k$ (0.17) reduces to the classical multistep formulas.
Up to now a linear stability theory for BVMs, which coincide to the classical one when $m = k$ has been completely derived. Two of the most important results are:

- existence of k-step 0-stable methods of order $2k$ for arbitrary k (disappearance of the first Dahlquist barrier)
- existence of A-stable methods of any order (disappearance of the second Dahlquist barrier).

When dealing with nonlinear problems the search of conditions that ensure the existence and uniquenesss of the solution of (0.17) becomes of primary importance.
We shall study here the unique solvability and convergence properties of (0.17) applied to problems which satisfy the one-sided Lipschitz condition

$$< \mathbf{f}(t, \mathbf{y}) - \mathbf{f}(t, \mathbf{z}), \mathbf{y} - \mathbf{z} > \leq \mu ||\mathbf{y} - \mathbf{z}||^2. \tag{0.18}$$

We derive sufficient algebraic conditions to have existence and uniqueness of the solution of (0.17), which only depend on the product $h\mu$. This will imply that for contractive problems ($\mu = 0$) we will have no restrictions as far as concerns the choice of the stepsize. The same conditions also answer the question whether the solution to the system of equations is stable with respect to perturbations and allow us to derive convergence results. As a further application, the obtained results will be also used to derive nonlinear stability properties of the classical multistep formulas without necessarily changing the method into its one-leg twin.

PARALLEL D: DIFFERENTIAL ALGEBRAIC EQUATIONS

On some New Stability Concepts for DAEs

G. Söderlind

Stability for DAEs is largely an open problem. So far, attempts have been made to adapt the usual stability notions for ODEs, such as Lyapunov stability and monotonicity conditions, to the DAE case. These concepts, however, have several shortcomings and are difficult to apply. In particular, the standard stability notions must be applied to an ODE on a manifold, the constraint manifold $\mathcal{M}$. When the DAE is discretized the numerical solution will normally not stay on the constraint manifold. It is therefore of interest to study the stability of solutions *outside* $\mathcal{M}$. The conventional approach of perturbing initial values cannot be applied to that situation as no solutions to the DAE exist outside $\mathcal{M}$.

In this talk we introduce some new stability concepts that permit solutions outside $\mathcal{M}$. Rather than perturbing initial values, we consider the effects of perturbing the equations, while the initial values are kept the same and consistent. The new concepts we study are modifications of L^p–stability, a well established notion in control and systems theory. Thus, given a DAE

$$F(t, x, \dot{x}) = 0\,; \qquad x(0) = x_0 \ \text{ consistent},$$

we consider the perturbed problem

$$F(t, x + \delta x, \dot{x} + \delta\dot{x}) = r\,; \qquad \delta x(0) = 0,$$

and ask that δx remain uniformly bounded for $t \geq 0$ when $r \in L^p$. More precisely, we say that the system is C^0/L^p–stable if

$$\forall \varepsilon > 0 \ \exists \delta > 0 \ : \ \|r\|_p \leq \delta \ \Rightarrow \ \|\delta x\|_\infty \leq \varepsilon,$$

where the norms are defined in the usual way.
This stability concept is directly related to the notion of perturbation index. For higher index systems, other spaces than L^p may be considered for the perturbation. For discrete systems, analogous definitions are made. The standard problem of considering what properties a discretization should possess for mathematical stability to carry over to numerical stability can then be studied.

We report on preliminary results and show by simple examples that the new stability concepts can discriminate between stability *on* $\mathcal{M}$ and *of* $\mathcal{M}$, respectively.

Stability Analysis in the Field of Industrial Applications

*P.A. Selting**

In the field of chip production, size and complexity of integrated electric circuits are permanently increasing. Nowadays circuit simulation programs are an important tool that gives information on the electrical performance of a circuit. In what follows, we refer to the simulation package TITAN, which has been developed at Siemens' research laboratories and is based on the well established simulator SPICE2.

Using Kirchhoff's laws and exploiting the constituting network element equations, a mathematical model is automatically built up in form of differential - algebraic equations, which is solved numerically. The solution characterizes the electrical behaviour of the circuit.

TITAN uses a charge oriented approach, which is closely related to the language of electrical modelling, for the basic algorithms and the formulation of the network equations. Unfortunately the equations are not given in symbolic form, but exist only in calculated form at discrete time steps.

A special task in simulation is the computation of limit cycles and the stability analysis of oscillating electric circuits. Periodic solutions play an important role in the design of electrical circuits. The question of stability arises, as in real life applications the parameters of the electric circuit like resistances, capacitances, ... depend on production tolerances for these elements. A loss of stability - caused by deviations of these parameters - means bifurcation and bifurcation is one of the main reasons for the irregular behaviour of a system.

We present a charge oriented approach for the investigation of local stability of limit cycles within the commercial simulation package TITAN. For that purpose the monodromy matrix has to be computed during the transient analysis phase and the dominant eigenvalues must be determined. This tool will offer the possibility to get information about the reliability of the electrical circuit.

For numerical tests we use industrially significant examples.

On Some Alternative Characterizations of Index in DAE's

M. A. Epton

The index of a differential-algebraic equation is a fundamental characteristic of the equation that is frequently needed by numerical software designed to solve such an equation. Three criteria for the determination of index will be presented. The first criterion states that a DAE of the form $\mathbf{f}(\dot{\mathbf{x}}, \mathbf{x}) = 0$ is of index 1 provided there is some selection of $n_1 = \text{rank}[\partial \mathbf{f}/\partial \dot{\mathbf{x}}]$ entries $\mathbf{f}_1, \mathbf{x}_1$ from $\mathbf{f}$ and $\mathbf{x}$ such that the following matrix is non-singular:

$$J_1 = \begin{bmatrix} 0 & \left[\frac{\partial \mathbf{f}_1}{\partial \dot{\mathbf{x}}}\right] \\ \left[\frac{\partial \mathbf{f}}{\partial \dot{\mathbf{x}}_1}\right] & \left[\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right] \end{bmatrix}$$

The virtue of this criterion is that it makes no assumptions at all about the structure of the DAE.

*The author is supported by BMFT: Federal Ministry for Research and Technology, project 3.0M250, project leader: Prof. Dr. R. Bulirsch and by the Siemens AG.

A second criterion, derived from the first, states that a DAE of the form,

$$\begin{aligned} \mathbf{f}_1(\dot{\mathbf{x}}, \mathbf{x}) &= 0 \\ \mathbf{f}_2(\mathbf{x}) &= 0, \text{where} \\ n_1 &= \dim[\mathbf{f}_1] = \operatorname{rank}[\partial \mathbf{f}_1/\partial \dot{\mathbf{x}}] = \operatorname{rank}[\partial \mathbf{f}_1/\partial \dot{\mathbf{x}}_1] \end{aligned}$$

is of index 2 provided $\mathbf{f}_2$ and $\mathbf{x}_2$ can be partitioned into pieces $\mathbf{f}_{2a}$, $\mathbf{x}_{2a}$ and $\mathbf{f}_{2b}$, $\mathbf{x}_{2b}$ of dimensions n_{2a} and n_{2b} respectively such that the following matrix is nonsingular:

$$J_2 = \begin{bmatrix} 0 & 0 & \left[\frac{\partial \mathbf{f}_1}{\partial \dot{\mathbf{x}}}\right] \\ 0 & 0 & \left[\frac{\partial \mathbf{f}_{2a}}{\partial \dot{\mathbf{x}}}\right] \\ \left[\frac{\partial \mathbf{f}_1}{\partial \dot{\mathbf{x}}_1}\right] & \left[\frac{\partial \mathbf{f}_1}{\partial \dot{\mathbf{x}}_{2a}}\right] & \left[\frac{\partial \mathbf{f}_1}{\partial \mathbf{x}}\right] \\ \left[\frac{\partial \mathbf{f}_2}{\partial \dot{\mathbf{x}}_1}\right] & \left[\frac{\partial \mathbf{f}_2}{\partial \dot{\mathbf{x}}_{2a}}\right] & \left[\frac{\partial^2 \mathbf{f}_2}{\partial \mathbf{x} \partial \mathbf{x}}\right] \dot{\mathbf{x}} \end{bmatrix}$$

The virtue of this criterion is that it avoids the fairly usual assumption that the DAE is in Hessenberg form and further explicitly illustrates the role of a second derivative tensor in determining the index of an index 2 DAE.

Finally a third criterion is *proposed* that the inverse of the Newton iteration matrix associated with the Backward-Taylor series of order m (denoted BT-m), when applied to an index k DAE, has a stable limit in its first $m - k + 1$ block rows. This criterion can be regarded as (yet another) definition of index. Results of numerical experiments will be presented indicating that this definition of index agrees with more conventional definitions of index.

Efficient Runge-Kutta Solvers for Index-2 Differential Algebraic Equations

J.C. Butcher[‡] *and R.P.K. Chan*

This talk considers the use of diagonal extensions to singly-implicit Runge-Kutta methods for the solution of index-2 differential algebraic equations (DAEs). The methods we discuss fall into two main classes. The first of these is based on the use of an $n \times n$ singly-implicit block to which are appended m further diagonally-implicit stages, as in Butcher and Cash [SIAM J. Numer. Anal. 27 (1990), 753-761]. In that paper, since stiff problems were the intended application, the appending of additional diagonally-implicit stages was motivated by a wish to include all stage abscissae within the overall step, but at the same time to preserve A-stability. In the DAE context, assuming that there is no stiffness, there is no need to demand good stability in the left half-plane but only at infinity. Hence, our aim here is to add the diagonally-implicit stages only for the purpose of improving performance of the method as a DAE solver.

In addition to standard singly-implicit methods, we consider a slight generalization originally proposed by Butcher [ACM Trans. Math. Software 14 (1988), 68-75]. In this generalization, the derivative of the solution used at the end of a previously completed step is used to obtain an order $n+1$ for the approximations produced in the $n \times n$ singly-implicit block with which the step commences. This is formally equivalent to regarding the method as having a first stage with zero abscissa placed before the $n \times n$ singly-implicit

[‡]This author's work was supported by the New Zealand Foundation for Research, Science and Technology.

block. For the purposes of our search for methods for index-2 DAEs, we will add $m (\leq 3)$ further stages after the singly-implicit block. If we interpret the method as having a preliminary explicit stage with abscissa 0, this will make a total of $n + m + 1$ stages.

For applications to index-2 DAEs of the form

$$y' = f(y, z), \quad 0 = g(y),$$

we derive stiffly accurate extended methods (respectively their generalizations) for the cases $m = 1, 2, 3$ having stage order n (respectively $n + 1$) with order $n + [(m + 1)/2]$ (respectively $n + m$) in y and order $n + [m/2]$ (respectively $n + 1 + [m/2]$) in z.

Defect-Based Error Controls for Index 2 and Index 3 DAEs

H. Nguyen

Consider solving a semi-explicit algebraic-differential equation

$$\begin{aligned} y' &= f(y, z), \quad y(t_0) = y_0, z(t_0) = z_0, \\ 0 &= g(y, z), \end{aligned}$$

and constructing interpolants u and v which satisfy the perturbed equation

$$\begin{aligned} u' &= f(u, v) + \delta, \quad u(t_0) = y_0, v(t_0) = z_0, \\ 0 &= g(u, v) + \theta. \end{aligned}$$

We propose an error control scheme which is based on the size of the defect D of an underlying equivalent initial value problem. By the Variation-of-Constants formula, we show that

$$u(t) - y(t) = \int_{t_0}^{t} \frac{\partial y}{\partial y_0}(t, s, u(s)) D(s, u(s)) ds,$$

and therefore controlling the size of D indirectly controls the global error of our approximate solution.

We applied this approach to a class of continuous projected Runge-Kutta methods. We were able to observe optimal continuous orders for these methods with an implementation based on sampling D at one point per step. An experimental code was implemented using the formulas Gauss(2), Gauss(3) and a second order diagonally implicit Runge-Kutta formula. Numerical results for index 2 and index 3 problems will be presented.

The Numerical Solution of Differential–Algebraic Systems by (m, k)-Methods

A.I. Levykin, E.A. Novikov

For the numerical solution of the initial value problem for systems of differential–algebraic equations a class of the so–called (m, k) - schemes is offered. The given class of schemes can be considered as the form of representation of a Rosenbrock type methods, in which a stage on a step of calculations is not connected with a compulsory calculation of the right part of a differential problem.

For (m, k) - schemes, the order equations are obtained in ase, when at calculations on stages we use the folloving:

a) time-lagged matrices of derivatives,

b) approximation matrices of derivatives.

There are obtained formulae of transition from the initial scheme to with respect to a part of parameters, that simplifies their investigation. At the number $k \leq 4$ of function evaluations of the right part of a differential problem the optimal in order of convergence (m, k) – schemes for systems, having an index not higher than two, are obtained.

Note, that in contrast to the case of the ODE systems, the order equations of (m, k) – schemes at realization in variants a) and b) are distinguished for differential–algebraic systems of index 1 beginning with the fourth order of accuracy and for systems of index 2 with of the third order of accuracy.

For (m, k) – schemes, the estimation of the global error is derived, and corresponding numerical algorithms are constructed. Results of numerical algorithms are presented.

Friday PM

PLENARY SESSION

Reversible Long–Term Integration with Variable Step Sizes

E. Hairer

This talk concerns the numerical integration of reversible (resp. Hamiltonian) systems by symmetric (resp. symplectic) Runge-Kutta methods. Special attention will be directed to the

- preservation of the geometric structure (invariants);
- long-term behaviour of the global error (linear error growth).

Much insight into these problems can be obtained by interpreting the numerical solution of an integration method formally as the exact solution of a perturbed differential equation (backward analysis) so that KAM theory can be applied.

In some situations (e.g., orbits with high eccentricity) it is desirable to work with variable step sizes. Classical step size strategies usually destroy the above mentioned properties. In the case of reversible systems a strategy will be discussed, for which the numerical solution preserves the geometric structure and has a linear error growth. This can be analyzed by extending the backward analysis of numerical integrators to variable step sizes. At the moment no similar strategy exists for symplectic methods and Hamiltonian systems.

The properties of symplecticness and of symmetry are very restrictive and the question arises whether it pays off to use such integrators in practical computations. Based on numerical experiments these questions will be studied. Comparisons between symmetric implicit Runge-Kutta methods and explicit extrapolation methods (applied with a more stringent tolerance) will be presented.

Most results of this talk have been obtained in collaboration with D. Stoffer. Related references are:

[1] M.P. Calvo & E. Hairer, *Accurate long-term integration of dynamical systems.* To appear in APNUM, 1995.

[2] E. Hairer, *Backward analysis of numerical integrators and symplectic methods.* Annals of Numerical Mathematics 1, 107–132, 1994.

[3] D.M. Stoffer, *Variable steps for reversible integration methods.* Manuscript. Submitted for publication, 1994.

New Runge-Kutta Schemes and Rosenbrock Methods

P. Shirkov

The history of the development of the numerical methods for the solution of the Caushy problem for the Ordinary Differential Equations (ODE) leaded to the construction of well-known schemes and computer codes (which are based on them). Among them there are the following ones: the classical Runge-Kutta method of the forth order, RKF4(5), DOPRI(4)5, DOPRI(7)8, ROS4A, RODAS, HW-SDIRK(3)4, STRIDE, LSODE, SEULEX etc. Their applications are very wide and they are used in the sphere from the simulation of the Mecanical Problems and the transient processes in Electric Circuits to the modelling of the fenomena in gases and polymers. Some of them are adapted to the problems of special type, for instance, to the stiff problems.

There is the question: is there any necessity to develop some new methods? One can give two different positive answers which supplement each other:

1. The construction of new methods and schemes relates to the pure theoretical interest.
2. It might improve classical codes and might give us new tools for the solution of complicated problems.

Both reasons enrich our knowledge of the theory and practice of the numerical methods.

In this article there are used some special requirements for the construction of the one step explicit and half-explicit methods for the solution of the Initial Value Problem (IVP) of nonstiff and stiff ODEs and there are constructed new schemes. Their advantages over well-known methods are illustrated with the use of generally accepted model problems.

Joint work with P. Kashcheev and K. Kochetkov.

PARALLEL 0: DIFFERENTIAL ALGEBRAIC EQUATIONS II

The main topic of this minisymposium are numerical methods directly applied to quite general index 2 differential-algebraic systems. In 1986, Bill Gear asked the question whether it is possible to cut down the numerical instabilities arising in higher index DAEs to certain subspaces as in the linear constant coefficient case. Now we are able to answer this question satisfactory for a quite large class of index 2 systems. On the background of a careful perturbation analysis of those equations, integration methods are discussed in detail (BFDs, Runge-Kutta methods, generalized projection variants, index checking, asymptotics etc.) by Arnold, Tischendorf, März.

In the same context, also numerical boundary value methods (e. g. multiple shooting) can be managed to work well for those index 2 systems. How to do that is proposed by Lamour, Petry. Chistyakov extends the discussion to include integral-algebraic systems.

Perturbations and the Numerical Solution of Higher Index DAEs

M. Arnold

The numerical solution of initial value problems for higher index differential-algebraic equations (DAEs) by straightforward discretization causes severe difficulties. Standard stepsize control algorithms from ODE theory have to be adapted to the DAE case, order reduction may occur and much effort has to be spent to solve systems of nonlinear equations that arise in the discretized equations. In addition to these problems in the practical realization of discretization methods trouble has to be expected since – in contrast to ODE theory – even the analytical solution of the initial value problem does not depend continuously on small perturbations in the DAE. The global error of a numerical solution that is actually computed contains not only the discretization error but an *additional error term* with errors that arise in the implementation of the method on a computer (e. g. errors caused by stopping the iterative solution of nonlinear equations, round-off errors). The additional error term may be very large for small discretization stepsizes h. This motivates the transformation of higher index DAEs into analytically equivalent ODEs or DAEs of index 1 *before* discretization.

The selection of efficient and reliable methods from the large set of index reduced and stabilized integration methods is very important from the point of view of practical applications. In the present talk we consider as one of the criteria for this choice the sensitivity of the numerical solution to small errors. Bounds for the additional error term in DAEs of index 2 and 3 are given that exploit the structure of the DAE. The additional error term is shown to be concentrated in some of the solution components (for systems in Hessenberg form: in the algebraic components). Stepsize control in variable stepsize codes can be based on solution components that are more robust against perturbations. Examples and numerical tests prove that the error bounds are optimal.

Various approaches to the numerical solution of model equations for mechanical multibody systems (that are of index 3) are compared w. r. t. their numerical effort and w. r. t. the robustness against perturbations. Simulation results for an example from railway system dynamics are presented. In contrast to the Euler–Lagrange equations for conservative mechanical systems that are considered most often in the literature this example leads to a DAE that is not in Hessenberg form and depends nonlinearly on the algebraic components (i. e. on the Lagrangian multipliers). The Gear–Gupta–Leimkuhler formulation of model equations for constrained mechanical systems is extended to this more complex example. The application of standard DAE solvers to this formulation yields to numerical methods that are both very efficient and robust against perturbations.

Recent Results in Solving General Index 2 DAEs

C. Tischendorf and R. März

The simulation of electric circuits is of a great interest today. The network equations obtained by the charge oriented modified nodal analysis lead to highly nonlinear DAEs with low smoothness properties. In general they do not belong to the class of Hessenberg systems studied in a lot of papers before.

On the background of a careful analysis of linear DAEs, linearizations of general nonlinear index-2 systems are considered. Finding appropriate function spaces and their topologies allows to apply the standard Implicit Function Theorem again. Both, solvability statements as well as the local convergence of the Newton-Kantorowich method (quasilinearization) result immediately.

The wide class of index-2 DAEs given here includes models of electric networks, for which the unique solvability was not known up to now. Further, the BDF applied to those general index-2 DAEs will be discussed to some extend. Also its asymptotic behaviour will be considered.

On The Numerical Treatment of Differential-Algebraic Systems and Their Integral Analogues

V. F. Chistyakov

This paper presents the results derived by investigating the systems of equations

$$F(x',\ x,\ Vx,\ t) = 0,\quad 0 < t < b, \tag{1}$$

where $x = x(t)$ is the n-dimensional desired vector-function, and V is the integral Volterra operator. The Jacobi matrix

$$\frac{\partial F}{\partial x'}$$

is assumed to be singular at all points of the domain of definition of F. Special cases of systems of the form (1) are differential- algebraic and integro-algebraic systems.

Solvability conditions for initial problems are formulated for the system (1) which ensure the validity of numerical methods. The most complete results are obtained for the linear case. A ring of linear integro-differential operators is constructed with a singular matrix at higher derivatives, in which the left-hand inverse operator is an operator of the same type.

Numerical methods both for investigating (calculating the index and checking for compatibility) and solving initial problems for the system (1) are considered. The methods of solution proposed in this paper are based on regularization and spline-collocation.

Two–Point Boundary Value Problems of Lower Index Differential Algebraic Equations

R. Lamour and T. Petry

Methods for solving DAEs basing on integration algorithms are presented. In the linear case, exploiting the linear structure, it is possible to apply the the transfer of boundary conditions due to Abramov and for the general implicit case a modified shooting method is introduced.

In the linear case the solution space of the DAE is represented by a set of algebraic equations, which are obtained by integrating a transformed version of the adjoint or dual problem. The so–called transfer equations are stable. Small perturbations of the right-hand side yield a regular perturbation of the inherent ODE of the given problem and, hence, a regular perturbation of the solution. The unique solution results by intersecting some affine subspaces calculated by the solution of an overdetermined system at every time step. In the general implicit case a clever combination of the calculation of consistent initital values and the shooting algorithm yields a system with a nonsingular Jacobian that has the same block–cyclic structure as for regular explicit differential equations. The calculation of the consistent initial values yields all the projectors needed for the shooting method.

Numerical examples are discussed.

PARALLEL A: EDUCATION ISSUES IN SCIENTIFIC COMPUTING

This minisymposium aims to stimulate discussions by presenting a broad ranging view of the educational needs and motivations in scientific computing and computational science and engineering. We will begin with an overview of academic programs currently in place in the U.S. These range from degree programs at the undergraduate as well as graduate level, as well as certificate programs. This is followed by the point of view of the future employer of students trained in this developing field. The government labs are the largest employers of computational scientists, but the private, high-tech sector also has their special needs. We will highlight one of the Department of Energy programs to support the development of undergraduate curricula in computational science. Then we finish with a presentation on the changing nature of education for this developing field.

An Overview of Academic Programs in Computational Science and Engineering

C.D. Swanson

Recognizing the need to educate science and engineering students in the methods of high performance computing, a growing number of universities are introducing computational science and engineering courses and programs. This talk will describe several representative computational science programs at the graduate and undergraduate levels and discuss trends in courses and curricula.

While computer science departments have been well established in our universities for many years, with a relatively well defined curriculum, computational science remains an interdisciplinary subject with an emerging curriculum, requiring the development of new courses not offered by traditional departments. Courses in four defined areas of computational science (applications, mathematics, computer science, and visualization) will be discussed.

The twenty-two graduate computational science programs included in this survey include eight that offer degrees in computational science, ten that offer specialty degrees (usually in the form of a minor or certificate) and four that offer graduate courses in computational science without any degree. Thus the trend in graduate computational science education is the specialty degree in which the student is part of a traditional science or engineering department (the "home" department) and meets additional requirements in computational science. These can include computational science and engineering courses and a computationally based thesis related to the home department's discipline. In addition, the student's examination committee may be required to include computational scientists. Upon graduation, the student receives an annotated degree, e.g., "PhD in Chemical Engineering and Computational Science."

The fifteen undergraduate computational science programs included in this survey include two that offer specialty degrees (minor or certificate) and thirteen that offer undergraduate courses in computational science without any degree. There are no undergraduate computational science departments or stand-alone degree programs. The undergraduate trend is toward interdisciplinary computational science courses supplementing existing course offerings.

Most of the current graduate and undergraduate computational science programs are at large research universities that own supercomputers or that have close associations with state or national centers. An issue for the near future is to extend computational science education into four-year liberal arts colleges and small universities. Network access to supercomputers and the availability of high-performance workstations and relatively low-cost departmental supercomputers provide opportunities for these schools to introduce computational science into their curricula.

A View from Government Laboratories on Training Computational Scientists

R.C. Allen

Sandia National Laboratories is a multi-program U.S. Department of Energy laboratory with major sites in Albuquerque, New Mexico and Livermore, California. Sandia's mission areas include national security, industrial competitiveness, energy resources and environmental quality.

High performance computing is already a key element of almost every major Sandia program, as well as programs at the other DOE laboratories. However, tremendous increases in computational capability, both hardware and software, are still needed for many applications. In the future, computer simulations must replace large-scale experiments that are no longer acceptable due to environmental consequences or costs. Simulations will also lessen dependence on expensive prototyping and retooling; entire systems will be computer simulated, redesigned, and optimized prior to actual assembly.

Some current application areas in high performance computing at Sandia include shock physics, computer design of materials, chemical reacting flows, low density flows, seismic processing, and medical imaging. Our recent highlights include: a series of Jupiter impact simulations alerted astrophysicists to the fact that fireballs would be visible when a series of comet fragments struck Jupiter last July; optoelectronics and catalysts with application-specific properties have been designed and optimized on high performance

computers; low density flow models have been used to analyze and optimize semiconductor manufacturing processes; and a Sandia-led industrial consortium is drastically reducing the time required to generate computational grids for unstructured finite-element calculations.

The Department of Energy is the Nation's largest consumer of computational scientists and engineers and, consequently, has a stake in insuring that there is an adequate supply of this human resource. The Department supports computational science activities and programs at the K-12, undergraduate, and graduate levels, as well as post-doctoral research opportunities in its laboratories. Several universities have now heeded the call, and "programs" in scientific computation are becoming more prevalent. The successful programs are interdisciplinary in nature, are oriented towards applications and problem solving, and use computation as an essential component.

In general, we would expect a computational science graduate to possess knowledge of applied mathematics and numerical methods; knowledge of and exposure to high-performance computing; general knowledge of computer science; knowledge in a science discipline; interest or experience in solving real problems; and the ability to interact in a team environment. Successful computational science activities are best accomplished by people with these qualifications working cooperatively in a team environment with applied mathematicians, and computer scientists. It is this environment that has contributed to the success of many of Sandia's programs in high performance computing.

An Industrial Perspective on Scientific Computing

D. Sulzbach

Genentech is a research driven Biotechnology company with approximately 2,500 employees. The Scientific Computing Department at Genentech supports the computing and information needs of corporate R&D activities. From my "Biotechnology industry point of view," scientific computing encompasses a much broader range of activities and requirements than is sometimes assumed.

"Scientific computing" at Genentech and other Biotechnology and Pharmaceutical companies includes computing activities from the very initial discovery of potential therapeutic agents to ultimate regulatory review and approval. This encompasses the computing and information needs of research scientists, assay developers and assay labs, preclinical testing, clinical testing, and regulatory submission. Although the specific details will vary from industry to industry, the general process of initial discovery, followed by testing and refinement, leading to ultimate development of a product that adheres to industry standards or regulations is common to most industries.

Because of the range of scientific activities at Genentech, scientific computing encompasses many things. Not all of these are typically identified as being part of "scientific computing." But, they are. During the past year, I and my staff have been involved in many activities, including the following:

- computational analysis and simulation (e.g., Computational Chemistry, Molecular Modeling, and structure refinement),
- designing and developing more efficient and user-friendly data management systems,
- facilitating access to and interpretation of electronic information resources,
- Bioinformatics,
- computer security,
- electronic documentation and document management,
- lab automation and robotics, and
- designing and developing Graphical User Interfaces to applications.

Future scientific computing activities at Genentech will be shaped by the following technology trends:

- increasingly powerful computers that are both affordable and supportable,
- faster and more widespread networks and their concomitant resources,
- Biological data bases that are growing rapidly in size and complexity,
- improving data storage and management technology, and
- digital imaging technology.

How well are students being prepared to work in this type of environment? In the last year we have hired 8 new full-time staff. Only one of these was hired directly out of school. She was in a graduate program in Computer Science. The others all had prior work experience. Without this experience, they would not have had the expertise and skills we needed.

I end with some personal observations and opinions. To wit:

- "Computational Science" is only one part of Scientific Computing.
- Data management is currently an underemphasized aspect of Scientific Computing.
- Universities will probably never be able to provide some of the information obtained from practical experience (e.g., "industrial strength" experience with commercial software for large document management).
- Computer security is becoming critically important to Scientific Computing in an industrial setting.

A Cooperative Volunteer Program for Undergraduate Curricular Materials

T. Marchioro

In the last 15 years the personal computer has been transformed from an exotic luxury into one of the common objects of modern living. Computers, and the services they provide, are becoming an inescapable part of the workplace; and the super-exponential growth experienced by the World Wide Web promises to make "computer literacy" a necessary trait for any member of a "well trained" workforce. Thus, I would seriously argue that an undergraduate student leaving college without significant hands on computer experience has not received an up-to-date (or perhaps even an adequate?) education.

The situation is even more pronounced in the sciences, where computers have become valuable research tools in all fields, and many now speak of a new, interdisciplinary, subject, "computational science", which treats computation itself as a means of scientific discovery. Clearly, anyone aspiring to be a modern research scientist must attain a degree of fluency with computers, and probably a working knowledge of "scientific computation" as well. However, despite the widespread evidence that computational literacy has become a requirement of most scientific research, organized efforts to teach these skills in the classroom have been largely limited to isolated efforts at individual schools and computing centers. If we as a society are to lead the transition to the information age, a coherent, well thought out, multi-institution approach to educating students in these matters is needed.

To address this need, the Department of Energy, through the Office of Scientific Computing, has initiated a set of educational projects in computational science. One of these, the Undergraduate Computational Engineering and Sciences (UCES) project, specifically promotes the incorporation of computation into the undergraduate curriculum. Over forty researchers and educators from the around the country have volunteered their time and effort to further UCES goals. Despite the widely varying backgrounds of UCES' members, a set of common experiences and desires emerged. I would like to present some of these shared experiences, and describe the actions UCES has taken to address them. These include:

1. A "core" set of concepts and techniques which any "computer literate" student should master must be identified. First and foremost, students must be presented with a variety of tools, including symbolic manipulators, procedural programming, visualization software, etc. and encouraged to choose the tool appropriate to the task at hand.
2. Advanced topics for the relative few who will pursue high end research or technical positions can also be addressed, but the emphasis should be on the mainstream.
3. Because computational science is a new field, new educational materials addressing the "core" issues must be developed and made readily available. Given the nature of the subject, it is most constructive if the materials themselves are provided "on-line". This approach also allows easy access by students and faculty at a wide range of institutions, not just research universities and supercomputing centers.
4. Educators themselves need easy-to-use tools authoring tools for creating suitable electronic materials. UCES has made significant progress in this regard.
5. A valid means of professional recognition must be provided so that educators are rewarded for addressing these issues. In order to implement a paradigm shift in how computers are used in education there must be tangible rewards for those who buck the "publish or perish" environment at research universities or take on an extra class at a liberal arts college or teaching school.
6. Other subjects, including our efforts at industrial outreach, as time allows.

Computational Science and the Changing Nature of Education

G.M. Johnson

The nature of Education is changing and Computational Science is helping to find the way into its future. The need for change in education is currently most evident in our public K-12 school system. It was set up to provide minimal skills to a large number of people so that they could participate fully in our society. It does deal with a large number of people, but the skills taught are out of synch with the times and the changed world situation. The very fact that the model for education is teaching rather than learning is indicative of the entrenched nature of the problems in K-12 education. The good news is that there is essentially universal agreement that K-12 education is "broken," and, consequently, it is fairly certain that it will soon be "fixed."

University education (including graduate education) remains fairly static in the U.S. There are a few notable exceptions where innovations are being implemented at the graduate level, but it is interesting to note that an undergraduate program in Computational Science is already in place at the National University of Singapore.

We believe that we are the best educators in the world; that we set the standards to which our competitors aspire; that we are a fixed point of reference in a changing world. We continue to believe all of this while our undergraduate schools are encountering increasing numbers of high school graduates requiring years of remedial help. Soon, assuming success in fixing the K-12 problem, universities may be overrun by students who cannot even relate to conventional teaching styles. They will have "learned" in K-12 and will not adapt well to being "taught" in higher education.

Successful learning involves openness, inquiry, experimentation, communication, collaboration, the absence of artificial disciplinary boundaries, and access to information and to expert advice and assistance. These are the attributes of Computational Science. In this talk I will make the case for Computational Science being a pathfinder into the future of Education.

PARALLEL B1: TRAJECTORY OPTIMIZATION

Trajectory optimization is a multidisciplinary process in which the design and control of a vehicle is analyzed. A trajectory optimal control problem includes the equations of motions, boundary conditions, path constraints, design constraints, and a performance index to be minimized. In this minsymposium, speakers will discuss the numerical solution of optimal control problems via multiple shooting and direct transcription (or collocation) techniques. Both multiple shooting and direct transcription approaches discretize the optimal control problem into a sparse, large-scale parameter optimization problem which is then solved with a nonlinear programmming algorithm. Topics to be addressed include multidisciplinary design optimization, optimal real-time guidance, and new results in large-scale, sparse nonlinear programming.

Optimal Interplanetary Trajectory Optimization By Direct Transcription

J. T. Betts

One of the most effective numerical techniques for the solution of trajectory optimization and optimal control problems is the direct transcription method. This approach combines a sparse nonlinear programming algorithm with a discretization of the trajectory dynamics. This paper describes the application of the transcription method to the solution of low thrust interplanetary orbit transfers. The vehicle dynamics are defined using a modified set of equinoctial coordinates, and the trajectory modeling is described using these dynamics. A solution is presented for a representative transfer from Earth to Mars, which includes a swingby of the planet Venus. This transfer serves to illustrate a number of features of the method which includes alternate coordinate systems during the transfer as well as mesh refinement to produce a high fidelity trajectory.

A Collaborative Approach To Trajectory Optimization

R.D. Braun and I.M. Kroo

The solution of large, coupled, multidisciplinary problems remains a challenging task in need of a flexible solution strategy. One potential solution strategy, which relies on the decomposition of a single, complex problem into numerous subspace optimization problems controlled through a coordination process, is termed collaborative optimization. Although applicable to many types of problems, collaborative optimization may be best suited for the large, sparsely-coupled problems often found in flight mechanics. These large, complex trajectory problems are difficult to solve with a single optimizer due to the large number of variables involved and nonlinearity of the design space. However, when posed in the collaborative framework, such a problem may be transformed into numerous solvable subproblems driven by a relatively small coordination process. In this presentation, the collaborative framework will be developed and demonstrated through the the solution of several trajectory optimization problems.

Application of Sparse Nonlinear Programming and Efficient Collocation to Optimal Guidance

C. Jaensch, M. Paus, and P. Gill

Recent advances in microprocessor technology now make it possible to consider optimal guidance approaches based on nonlinear programming (NLP) techniques for implementation in future air- and spacecrafts. What makes optimal guidance schemes based on nonlinear programming so attractive compared to other approaches is their inherent flexibility in the problem formulation. In principle almost arbitrarily complex optimal control problems can be formulated and it is just a matter of the available computer resources and the quality of the appropriate solvers whether these problems can be solved in real-time to be utilized in a guidance law. Practical experience has shown that there are mainly four requirements that have to be met by the underlying trajectory optimization method: speed – reliability – large convergence radius – smoothness of the resulting control history. The requirement for a high reliability and a large convergence radius makes the direct collocation method an attractive candidate, whereas the speed requirement favors a shooting or multiple shooting approach. Since the collocation approach results in a relatively large number of parameters which are locally highly constrained, it yields in combination with most "off the shelf" (dense) NLP solvers excessive computation times. Thus, if one wants to exploit the positive properties of collocation one has to address this performance problem. Two measures are presented that allow a reduction of the computation time to a real-time guidance requirements level.

As a first step, the sparsity of the constraint derivatives (the Jacobian) is exploited in the NLP solver. The discretized problems are solved using the general-purpose package SNOPT (Sparse Nonlinear OPTimizer), which is the implementation of a sequential quadratic programming (SQP) method. SNOPT treats the Jacobian as a sparse matrix and works with a reduced Hessian. This reduced-Hessian approach is effective whenever the number of constraints active at the solution is similar to the number of variables. For efficiency, the difference may be anything from zero to a few hundred. Two features of SNOPT make it particularly well suited to guidance problems. First, the quasi-Newton reduced Hessian may be replaced periodically by a finite-difference Newton approximation. This improves the rate of convergence and allows the rapid exploitation of a good starting point. The second feature of SNOPT is that the reduced Hessian may be larger than the current number of superbasic (or "driving") variables. (We say it has a "border".) For cases in which no good estimate of the solution is known, the border can be relatively large—with a corresponding increase in robustness. By contrast, if a good estimate of the solution is available, a small or zero border will usually suffice—with a corresponding decrease in computation time.

The enormous speed up achieved with SNOPT in an existing collocation code revealed that the function and derivative evaluation is now the performance bottleneck, consuming 60-85% of the total computation time. Thus as a second step, a more efficient formulation and implementation of the collocation scheme has been derived. In this formulation the linearized system dynamics are explicitly utilized to permit an extremely efficient evaluation of all collocation constraints and more importantly the associated sparse Jacobian. This formulation has been tested on a 3-dimensional minimum time intercept maneuver, where the linearized system dynamics of the aircraft model were given analytically. The results show that first of all, the function and derivative evaluation time could be reduced for this test problem to approximately 30% of the total computation time. Secondly, a full trajectory optimization with a moderate discretization of 16 nodes can be performed from a rather crude starting estimate within the targeted 1-2 seconds on a 12 MFlops computer—the minimum expected performance of a future on-board processor.

Structured Interior Point SQP Methods

M.C. Steinbach

Trajectory optimization is an important means to improve performance in many industrial and scientific processes such as robotics or aerospace applications. A combination of SQP methods with direct collocation or multiple shooting discretizations has proven very successful for such problems. In realistic applications, however, very large QP subproblems with thousands of constraint may arise. The lecture presents an approach based on highly efficient solution of the block-sparse QP by a structured Interior Point method.

Accuracy Refinement in Direct Transcription Methods

K. Brenan

This talk will focus on current strategies used in direct transcription software for controlling the accuracy of the numerical solution of trajectory optimal control problems. In the direct transcription approach, the optimal control problem is discretized by a collocation formula into a sparse, large-scale parameter optimization problem. Then a nonlinear programmming algorithm is used to determine the optimal discretized solution which includes numerical approximations for the state, the control, and the adjoint variables at a set of mesh points. Accuracy refinement may be achieved in a variety of ways. Methods currently being employed in direct transcription codes, such as mesh refinement, deferred correction, and bi-level optimization, will be discussed. The effectiveness of these error measures in controlling the accuracy in the objective function value and the state, control, and the Lagrange multiplier estimates of the adjoint variables will be assessed. To conclude the talk, numerical results of some accuracy refinement experiments will be presented.

PARALLEL B2: SPECIAL SECOND–ORDER ODEs

Nonlinear Smoothing for Highly Oscillatory ODEs

C. Schütte

Nonlinear ODEs with highly oscillatory solutions are a subject of much actual interest today. They appear in many concrete applications from electronic curcuit simulation, multibody dynamics, or quantum chemistry, for example. The fast oscillations of the trajectories confine the stepsizes of any numerical integrator. In most real life problems this causes a tremendous computational effort. The efficiency of the simulations can only be increased by avoiding the evaluation of all the oscillatory details, i.e. by computing *smoothed* or *averaged* trajectories, only.

For this purpose, different well-known *linear* smoothing techniques have been developed, e.g. averaging or filtering methods. But although these techniques are successful in many situations, there are important cases in which they are simply inappropriate. These are cases in which the dynamic of the system is

essentially nonlinear, forcing us to use also *nonlinear* smoothing techniques. Typical examples are problems from molecular mechanics (large systems) and time–dependent quantum chemistry (nonautonomous systems).

For some particular situations, specific nonlinear "smoothers" have been constructed, mostly in the framework of perturbation analysis. But nevertheless, the theoretical background for a generalization is still missing. This talk will give examples for the problems and methods named (including the presentation of a typical nonlinear smoothing technique in the presence of resonance effects [1]) and will present an interesting proposal for the aspect of generalization.

[1] *A quasiresonant smoothing algorithm for solving large highly oscillatory differential equations from Quantum Chemistry*, Konrad–Zuse–Center, Berlin, TR 94-4, 1994.

Fourth Order P-stable Block Method for Solving the Differential Equation $y'' = f(x, y)$

K. Ozawa

A certain type of P-stable block method of order 4 is derived for solving the second order initial value problem $y'' = f(x, y)$. The block method considered here consists of two P-stable linear multi-step methods and computes the numerical solutions at the two points of x simultaneously. Moreover some technique to reduce the local truncation error of the method is developed.

PARALLEL C1: ODEs IN CHEMICAL AND ATMOSPHERIC SCIENCES

Many models in atmospheric and chemical sciences are described mathematically by systems of partial differential equations. The discretization of the spatial derivatives involved in these systems leads to huge systems of ODE's, which must normally be treated numerically over long time-intervals. This means that many time-steps have to be performed.

Moreover, the systems of ODE's arising from the chemical sub-models are very often both stiff and badly scaled. Photochemical reactions are switched on after sun-rise and switched off after sun-set. This leads to very quick changes of the concentrations of some chemical species in the periods of sin-rises and sun-sets. Therefore it is very difficult to design numerical methods which can efficiently handle such huge stiff systems of ODE's.

The systems of ODE's which arise after the discretization of the advection-diffusion sub-models are as a rule not very stiff. However, also here sharp gradients of the concentrations occur very often. Therefore also these systems are rather difficult.

It is important, in many models at least, to couple properly the chemical and the advection-diffusion sub-models. This is normally the most difficult part of the work. The fact that both the numerical algorithms used in the advection-diffusion sub-model and the numerical algorithms used in the chemical sub-model are sufficiently accurate and sufficiently fast does not automatically mean that the combined numerical

algorithm has also these properties. Therefore careful tests of the performance of the global algorithm are absolutely necessary.

Finally, the systems of ODE's are, as mentioned above, very large. It is not uncommon that systems containing up to several millions of equations are to be treated during several thousands of time-steps. Therefore high-speed computers are to be used in the numerical treatment of large-scale atmospheric and chemical problems. It is rather diffucult to develop an efficient code, because one has to manipulate with very large data files and to unite and optimize different computational processes.

Several promising solutions of the challenging tasks that have been listed here will be discussed in the talks that will be presented at this symposium.

Fast UAM: an Example of an Adaptive Approximation Solver for Atmospheric Chemistry Problems

P.D. Guthrie, G. Yarwood, S.B. Shepard and M.P. Ligocki

Models of atmospheric photochemistry must address the problem of repeatedly solving a stiff, non-linear coupled system of differential equations for a large set of chemical species. The stiffness of the system may vary greatly during the course of a simulation. Classical stiff solvers (e.g., Gear's method) have proven prohibitively expensive for use in operational atmospheric chemistry modeling. In response a number of approximate methods have been developed. Some, such as QSSA and the Hybrid method, can be very fast, but can also become wildly inaccurate under some conditions since they neglect the off-diagonal terms of the Jacobian entirely. Others, such as the Urban Airshed Model (UAM) solver and the recently developed Implicit-Explicit Hybrid (IEH) method retain the coupling of a reduced set of species, but assume that limiting approximations hold for either the short-lived (UAM steady state) or long-lived (IEH explicit) species. These latter methods are still computationally burdensome in operational applications, where many simulations must be carried out.

We present a modified UAM solver, termed the Fast UAM, which employs the concept of adaptive approximation to modify the solver algorithm depending on local conditions during the course of the calculation. The method divides the chemical species into three classes: steady state (time constants always much shorter than a time step), slowly varying (time constants always much longer than a time step) and intermediate. The intermediate species constitute a very small system (typically 3 or 4 species) which can sometimes be well approximated by simple analytic expressions, and must sometimes be solved by a technique such as Newton-Raphson iteration. This decision is internally coded and made on the fly.

Speed and accuracy performance tests of this solver in box model and full grid model applications will be presented. Testing issues appropriate to this and other application-specific solvers will also be discussed.

Finite Element Approximation of Large Air Pollution Problems I: Advection

B. Neta

A finite element method for the solution of the two dimensional advection equati on was developed. Bilinear rectangular elements were used. Linear stability anal ysis of the method is given.

An Implicit-Explicit Approach for Atmospheric Transport-Chemistry Problems

J. Verwer

Transport-chemistry problems take into account a variety of physical processes. From the numerical point of view, three important processes are the constituents exchanges due to stiff chemical reactions, advective transport, and vertical transport caused by turbulent diffusion. In practice the numerical treatment of the stiff chemistry turns out to dominate CPU costs. Since atmospheric chemistry is still in development, and more and more reactions between more and more species are included, numerical research into efficient algorithms and software for atmospheric transport-chemistry models is of interest.

For stability reasons, stiffness normally impedes the use of implicit time-stepping techniques combined with modified Newton iteration for computing the implicitly defined solution. In [2,3] we have shown, in a box model computation and using the implicit 2nd-order BDF method, that for atmospheric chemistry problems a simple Gauss-Seidel method can be used. This is attractive since in this way the numerical algebra overhead of a Newton method can be avoided and much less storage is needed. In fact, the Gauss-Seidel method used is truly explicit and related to the simple, explicit quasi-steady-state-approximation (QSSA) approach to which it compares very favourably [3].

In the lecture we will further explore the Gauss-Seidel technique for a 2nd-order implicit-explicit BDF-type integration scheme which treats advection explicitly and the stiff chemistry and vertical diffusion implicitly. This implicit-explicit scheme is derived along the method of lines and can be applied with variable stepsizes similar as in [2,3]. For the discretization of the spherical advection operator we employ the mass-conservative, flux-limited finite-difference scheme discussed in [1]. This scheme is based on the 3-rd order upwind biased method which is equivalent to the kappa=1/3-scheme of van Leer and found to be very suitable for our application. The Gauss-Seidel technique is used for the coupled solution of chemistry and vertical diffusion, in a manner that for the diffusion the implicitness is retained, whereas for the chemistry the computation is explicit, similar as in the box model case.

[1] W.H. Hundsdorfer, B. Koren, M. van Loon, J.G. Verwer, *A positive finite-difference advection scheme*, J. Comput. Phys., to appear in 1995

[2] J.G. Verwer, *Gauss-Seidel iteration for stiff ODEs from chemical kinetics*, SIAM J. Sci. Comput. 15, 1243 - 1250, 1994

[3] J.G. Verwer, D. Simpson, *Explicit methods for stiff ODEs from atmospheric chemistry*, Appl. Numer. Math., to appear in 1995

Treatment of Stiff and Badly Scaled ODE Problems in Large Air Pollution Models

Z. Zlatev

Studying the transboundary transport of air pollutants is an important environmental problem. Systems of partial differential equations are normally arising when mathematical models are used in the solution of this problem. The interrelations between the different air pollutants are rather complicated. Therefore many air pollutants are to be included in the models. This leads to very large and very complicated numerical tasks. The chemical part of an air pollution model is one of the most difficult parts for the numerical algorithms. It is necessary to apply reliable and sufficiently accurate algorithms during the numerical treatment of the chemical sub-models. Moreover, it is also necessary to apply fast numerical algorithms that can be run efficiently on the modern high-speed computers. These two important requirements work, as often happens in practice, in opposite directions. Therefore a good compromise is needed. Some results achieved in the efforts to find a good compromise will be described. The advantages and the disadvantages of several numerical methods will be discussed. All conclusions are made for the particular situation where large air pollution models are to be treated on big modern high-speed computers. Moreover, it is also assumed that a particular air pollution model, the Danish Eulerian Model ([1], [2]), is used. However, the ODE systems that arise in the chemical sub-models have at least three rather common properties, which appear again and again when large scientific and engineering problems are studied. These systems are large, stiff and badly scaled. Therefore some of the conclusions are also valid in a much more general context, i.e. in all cases where large, stiff and badly scaled systems of ODE's are to be handled numerically.

[1] Z. Zlatev *Numerical Treatment of Large Air Pollution Models*, Kluwer Academic Publishers, Dordrecht-Boston-London, 1995
[2] Z. Zlatev, I. Dimov and K. Georgiev *Modelling the Long-range Transport of Air Pollutants*, Computational Science and Engineering, Vol. 1, No. 3 (1994), 45–52.

Exact Solutions to Turbulent Particle Laden Flow Equations

McKee

An understanding of disperse particle flow and deposition are important for safety studies in the Nuclear Industry, flow and deposition from chimneys, hairsprays, and corrosion. Probability density function equations have proved very useful in studying the behaviour of such stochastic systems; obvious examples of their usage occur in the study of Brownian motion and in the kinetic theory of gases. This talk will focus on a Boltzmann type equation for particle laden flows developed by Reeks and his co-workers in a series of papers in J. Fluid Mech. and Phys Fluids. First two techniques for solving a certain class of partial differential equations are developed and then used to provide exact solutions to the Reeks' equation. In particular, they are applied to flows subject to simple shear.

PARALLEL C2: METHODS FOR STIFF ODEs

Experiences with a Stiff ODE-Solver Based on Automatic Differentiation and Rational Approximation

H.J. Stetter[§]

For IVPs of nonlinear systems of ODEs $y'(t) = f(t, y(t))$, automatic differentiation permits an automated computation of arbitrarily long expansions of the Jacobian along the solution trajectory through a specified point (t, y). This suggests the design of high-order predictors for the associated "linear" systems for $z(t) := y'(t)$

$$z'(t) = J(t, y(t)) \cdot z(t)$$

which are based on rational approximations for z. For stiff systems, such predictors produce accurate values of z over long step if the Jacobian does not vary too violently along the trajectory, i.e. outside transient domains with strong nonlinearities. Corresponding high order rational predictors may then be used for the accurate approximation of the trajectory.

After a short explanation of the method and the code, results for various types of nonlinear stiff systems will be presented and discussed. We will identify the classes of problems for which this approach appears more efficient than state-of-the-art approaches.

QSSA Integrators for Stiff ODEs arising in Computational Atmospheric Chemistry

F. Potra

More than 90% of the computational time of existing regional- and global-scale atmospheric chemistry and transport models is spent in numerical integration of the (very) stiff system of ordinary differential equations describing chemical kinetics. This integration has to be performed for long time horizons - from several hours to several months. The actual codes run in "real time" for 3-D simulation one workstations (one day requires 24 hours computer time on an HP workstation!), and predictions based on such codes require heavy supercomputer use.

The Quasi-steady-state-approximation (QSSA) scheme has become the standard integrator in this field in the last 15 years. This method is, for atmospheric chemistry problems, more effective than general stiff ODE solvers. It takes advantage of the structure of the problem and of the low accuracy requirements. Many efforts have been made to improve QSSA, but most of the new schemes are based on a specific chemistry mechanism rather than on general mathematical principles, and therefore, they cannot be applied directly to new situations. Moreover, since these methods are difficult to vectorize and/or parallelize, they may be less efficient on machines with a large number of (vector) processors.

We develop and analyze some QSSA-based schemes, in an attempt to improve both speed and accuracy. The research was carried along two main directions : extrapolation and multistage QSSA. Among them, the new Symmetric QSSA seems to perform best. It allows the computational time to be halved, while keeping the relative error in the range of 5%. For smaller errors, this new method is seven to ten times faster than the standard QSSA.

[§]joint work with G. Corliss, A. Griewank, P. Henneberger, F. Potra, G. Schranz-Kirlinger

PARALLEL D1: ODE METHODS IN PDEs

Variable Order Spatial Differentiators in the Method of Lines

W. Schiesser

Adaptive Finite Element Methods of Lines with Applications to Materials Processing

J. Flaherty

Some ODE Problems associated with Moving Node Methods

K. Miller

A Moving Collocation Method and some Applications

W. Huang

An Introduction to Adaptive Method of Lines and Its Related ODE Issues

R. Russell

PARALLEL D2: BOUNDARY–VALUE METHODS FOR INITIAL–VALUE ODEs II

A Cyclic Reduction Approach to the Numerical Solution of Boundary Value ODEs

P. Amodio and M. Paprzycki

Most of the discretization methods for Boundary Value ODEs (as well as some methods for DAEs) lead to the creation of Almost Block Diagonal (ABD) linear systems. Depending on the particular discretization method, boundary conditions (separated or not), number of ODE's and their degrees as well as on the number of discretization steps, there exist several methods for efficently solving these linear systems on

parallel computers.

In [1] we considered a parallel algorithm tailored for distributed memory computers for the solution of ABD systems arising from BVPs with separated boundary conditions. This solver allowed us to reduce the computational cost and the memory requirement in comparison with some other known solvers. In our presentation we will show how to combine this factorization with generalized cyclic reduction in order to obtain a parallel solver that makes possible the solution of linear systems arising from BVPs with non-separated boundary conditions.

We discuss the arithmetical complexity and the storage requirement of the new algorithm as well as the parallel implementation details.

[1] P. Amodio, M. Paprzycki, *A parallel solver for almost block diagonal systems on distributed memory computers*, Presented at the Fourth Conf. of the Intern. Linear Algebra Society, August 15–19, 1994, Rotterdam, The Netherlands.

On Optimally Scaled Systems for Second Order Scalar Singularly Perturbed Problems

L.V. Kalachev and Robert M.M. Mattheij

The conditioning of singularly perturbed scalar Dirichlet problem is considered. It is shown how this is related to the conditioning of an appropriate associated first order system. Two typical equations are studied in more detail, one with possible boundary layers on both sides of the interval and one with the internal layer (turning point case). The results are applied to obtain estimates of global discretization errors for difference methods.

Saturday AM

Software for ODEs

L.F. Shampine

The talk will begin with memories and opinions about the development of mathematical software, esp. software for initial value problems for ODEs, since 1960. Current developments will be exemplified by the speaker's work on a suite of ODE codes for MATLAB and a multimedia project for the teaching of ODEs with computer experiments.

Cedar: An Experiment in Parallel Computing

A. Sameh

The Cedar multiprocessor project started at the University of Illinois at a time of intense activity in the parallel processing community. The main topics were, and still are, the evaluation of different architectures and their effectiveness in handling large-scale applications in science and engineering. A multidisciplinary center was established to build this multi-cluster shared-memory multiprocessor, design and implement the associated system software and the mathematical libraries, as well as measure the performance of the whole system on a variety of applications. This paper gives an overview of the research and development effort which lasted roughly seven years ('85-'91), with emphasis on the parallel numerical algorithms designed for a variety of applications. The results obtained from this experiment have been of use to similar efforts in industry and few academic institutions. Another important byproduct of this project has been the recognition of the need of an educational program in Computational Science and Engineering.

ODEs are not OLDIEs. Current Views and Activities

P. Deuflhard

The talk will address numerical analysis of ODEs from the point of view of *dynamical systems*. First, in a conceptual introduction (following a recent textbook of DEUFLHARD/BORNEMANN), the condition number of an IVP solution versus the *discrete condition numbers* of its one–step or multistep numerical counterparts will be discussed. From this, some view on *stiffness* will naturally emerge, which even applies for a scalar ODE. A–stability will be interpreted in the analytical frame of hyperbolic dynamical ODE systems.

This does not cover the dynamics on center manifolds, which therefore deserve special attention in the second part. Apart from symplectic discretizations of Hamiltonian systems, which will be covered by other speakers, *smoothing techniques* for highly oscillatory ODE systems will be focussed. The dynamical systems point of view clearly favors *nonlinear* smoothing techniques rather than the traditional linear ones. Problems of this kind arise all over computational quantum mechanics, when time–dependent Schroedinger equations have to be solved (see SCHÜTTE). In the third part, recent numerical techniques for hyperbolic ODE systems will be analyzed. Dynamical sparsing of the Jacobian (due to NOWAK) appears as a rather simple heuristic in the context of linearly implicit one–step methods, especially useful for compartment models. Finally, *approximate inertial manifolds* will be carefully studied in view of their efficiency in actual ODE computation. One decisive issue is the choice of basis, a second one is the selection of the number of degrees of freedom. In most present realizations, a fixed dimension of the AIM is selected. Methods of this structure are of some help in real life combustion computations (cf. MAAS/POPE), but also show certain pitfalls. As a remedy, a *dynamical control of the dimension* is suggested, which, however, may not be easy to implement in a PDE context – the true aim of AIM.

Yes, there was something left to do

J. C. Butcher

In his well-known 1981 paper, Bill Gear asked a question in the title, "Numerical solution of ordinary differential equations: is there anything left to do?" Although no one could have given a more authoritative answer to this question than he gave, different answers could also have been given. With the benefit of hindsight, some of the things which Bill felt still needed to be done, and also other things he might possibly have proposed, will be reviewed in the present survey lecture. Some of the specific questions to be asked will be

- did the things Bill discussed really need to be done?
- have they now been done?
- were there other things that needed to be done?
- have these also been done?
- what things to be done have come to light since 1981?

Of course the central question is now, as it was then: "To what extent is numerical ordinary differential equations still a fertile research area?" This lecture is my personal answer to this question.

Saturday PM: GEAR FESTIVAL

Computer Simulation of Biomolecules and the Real Error of Symplectic Integrators

R.D. Skeel

In some applications, like molecular dynamics, the ODEs are unstable, and detailed accuracy in the trajectory is unattainable over significant intervals of time. For such problems it seems quite useful instead to look at the error in the "modified ODE"—the ODE which is exactly satisfied by numerical trajectories. However, difficulties are encountered in this approach, which leads to the idea that the numerical solution should not be taken at face value but rather be regarded as a slightly corrupted version of a hidden numerical trajectory. Stated less dramatically, it is shown for Hamiltonian systems how a combination of forward error analysis with backward error analysis might lead to a more meaningful assessment of accuracy.