Final Program

Advances and Challenges in Time-Integration of PDE's

Location:
Barus & Holley Building, Room 190,
Division of Engineering
182 Hope Street, Providence

Brown University
Division of Applied Mathematics
August 18-20, 2003

Workshop sponsored by Air Force Office of Scientific Research

SCHEDULE FOR WORKSHOP

Monday, August 18, 2003

TIME	SUBJECT/SPEAKER/TITLE	SESSION CHAIRMAN
8:00-8:15	Coffee/Juice/Registration	
8:15-8:30	Welcoming remarks by C. Rhoades, AFOSR	
8:30-9:30	J. Butcher, Univ of Auckland, New Zealand *High order A-stable numerical methods for stiff problems*	C. Rhoades, AFOSR
9:30-10:00	Coffee Break/Registration	
10:00-11:00	E. Hairer, Univ. Geneve, Switzerland *Important aspects of geometric numerical integration*	W. Hilbun, AFOSR
11:00-12:00	L. Shampine, Southern Methodist Univ., TX *Error estimation and control for ODEs*	
12:00-1:30	Lunch break	
1:30-2:30	A. Jameson, Stanford University TBA	M. Carpenter, NASA LaRC
2:30-3:30	R. Elman, U. Maryland, College Park *Preconditioning strategies for models of incompressible Flow*	
3:30-4:00	Coffee Break/Registration	
4:00-5:00	C. Woodward, LLNL TBA	
5:00-6:00	D. Knoll, LANL *Jacobian-Free Newton-Krylov methods for the accurate time integration of stiff wave problems*	
6:30-8:00	**Reception in the Brown Faculty Club**	

Tuesday, August 19, 2003

TIME	SUBJECT/SPEAKER/TITLE	SESSION CHAIRMAN
8:00-8:30	Coffee/Juice/Registration	
8:30-9:30	Z. Jackiewicz, Arizona State *Construction and implementation of general linear methods for ordinary differential equations*	J.S. Hesthaven, Brown
9:30-10:00	Coffee Break	
10:00-11:00	U. Ascher, Univ. British Columbia, Canada *Symplectic and multisymplectic methods for the KdV equation?*	
11:00-12:00	J. Verwer, CWI, The Netherlands *On solving highly stiff diffusion-reaction systems*	
12:00-1:30	Lunch break	
1:30-2:30	S. Thomas, NCAR *The NCAR spectral element climate dynamical core: Semi-implicit, semi-Lagrangian formulation*	D. Gottlieb, Brown
2:30-3:30	G. Karniadakis, Brown TBA	
3:30-4:00	Coffee Break/Registration	
4:00-5:00	B. Gustafsson, Univ of Uppsala, Sweden *High order time compact difference methods for wave propagation problems*	
5:00-6:00	J. Shang, Wright State/AFRL *Time scales and solving schemes of Computational Magneto-Aerodynamics*	
7:30–>	**Conference Dinner** Capriccio Restaurant 2 Pine Street Providence, RI 02903	

Wednesday, August 20, 2003

TIME	SUBJECT/SPEAKER/TITLE	SESSION CHAIRMAN
8:00-8:30	Coffee/Juice/Registration	
8:30-9:30	Y. Kevrekidis, Princeton University *Equation-free multiscale computation: Enabling microscopic simulators to perform system level tasks*	B. Gustafsson, Uppsala
9:30-10:00	Coffee Break	
10:00-11:00	G. Russo, University of Catalania, Italy *Implicit-explicit Runge-Kutta schemes and applications to hyperbolic systems with relaxation*	
11:00-12:00	S. Gottlieb, UMass/Dartmouth TBA	
12:00-1:30	Lunch	
1:30-2:30	H. Najm, Sandia NL *Time-integration of low Mach number reacting flow with detailed chemical kinetics*	S. Abarbanel, Tel Aviv
2:30-3:30	J. Bell, LBL *Temporal discretization methods for reacting flows with detailed chemistry*	
3:30-4:00	Coffee Break	
4:00-5:00	M. Carpenter, NASA Langley *Fourth-Order ESDIRK schemes for fluid mechanics applications*	
5:00-6:00	R. Temam, Univ d'Orsay, France Cancelled	

Symplectic and multisymplectic methods for the KdV equation?

by

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Abstract

The design and development of symplectic methods for Hamiltonian ordinary differential equations (ODEs) has often yielded very powerful numerical schemes with beautiful geometric properties. Symplectic and other symmetric methods have been noted for their superior performance, especially for long time integration. On the other hand, it has long been known that conservative discretization methods for nonlinear, nondissipative partial differential equations (PDEs) governing wave phenomena tend to become numerically unstable, especially for long time integration. Thus, the common beliefs of two established communities seem headed to a clash upon examining symplectic time discretizations for Hamiltonian semi-discretizations and multisymplectic discretizations of certain Hamiltonian PDEs.

We therefore examine some symplectic and multisymplectic methods for the notorious KdV equation with the question whether the added structure preservation that these methods offer (at a price) is key in providing higher quality methods for such problems. Please stay tuned for the answer.

High order A-stable numerical methods for stiff problems

by

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Abstract

The only way to obtain high order A-stable methods is by having many stages of calculation in each time step. Let A denote the coefficient matrix relating the stage values to the stage derivatives. To lower implementation costs, specific structures for A have to be insisted on. We consider singly-implicit Runge-Kutta methods for which $\sigma(A) = \{\lambda\}$, with λ chosen by stability criteria and general linear methods which possess the stronger property that A is lower triangular with constant λ on the diagonals. This talk is an overview of these two types of method with special emphasis, in the Runge-Kutta case, to effective order and, in the general linear case, to inherent RK stability.

Fourth-Order ESDIRK schemes for Fluid Mechanics Applications

by

Mark Carpenter
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Abstract

Recent experiences with Explicit Singly Diagonal Implicit Runge-Kutta (ESDIRK) schemes are presented in the context of high Reynolds number, turbulent flows. Structured and unstructured codes are used to compare the ESDIRK schemes with the BDF2, BDF3 and MEBDF4 schemes. Cost comparisons are made at different precisions, and the effects of order-reduction is quantified. Critical areas are identified for future work.

Preconditioning Strategies for Models of Incompressible Flow

by

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Abstract

We describe some new preconditioning strategies for handling the algebraic systems of equations that arise from discretization of the incompressible Navier-Stokes equations. We show how these approaches relate to classical techniques such as projection methods and SIMPLE, demonstrate how they adapt in a straightforward manner to decisions on implicit or explicit time discretization, and explore their use on a collection of benchmark problems.

High order time compact difference methods for wave propagation problems

by

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Abstract

It is well known that wave propagation problems over long time intervals require high order methods, and many such methods have been constructed. However, to keep high order accuracy also in time for problems with variable coefficients and minimal storage, the methods quickly become complicated. In this talk, we will consider acoustic wave propagation, and discuss a few finite difference methods for the wave equation in scalar form as well as in first order system form.

One way to achieve high accuracy in time, is to use Taylor expansion and substitute time derivatives by space derivatives by using the differential equation. It turns out that the first order system form leads to less complicated approximations, while still keeping the conservation properties of the continuous formulation. We will show that the method works well even for discontinuous coefficients without any special procedures across the material interfaces.

The deferred correction principle is well known for obtaining high order accuracy in space, but it can also be used in the time direction. We will present some new results for this type of methods based on implicit time discretization of first order PDE systems. By slightly weakening the stability concept, it is possible to keep the unconditional stability even for the higher order methods.

Important aspects of geometric numerical integration

by

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Abstract

A short review about properties and advantages of symplectic, symmetric and reversible methods for the numerical integration of Hamiltonian systems will be given. The emphasis is on aspects that are important but sometimes overlooked, such as: existence of globally defined modified Hamiltonian, limits of backward error analysis, use of variable step sizes. Numerical phenomena will be reported that still miss a theoretical explanation.

Construction and Implementation of General Linear Methods for Ordinary Differential Equations

by

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Abstract

In the first part of this lecture we will give the overview of different approaches to the construction of diagonally implicit multistage integration methods for both nonstiff and stiff differential systems of ordinary differential equations. The identification of high order methods with appropriate stability properties requires the solution of large systems of nonlinear equations for the coefficients of the methods. For low orders these systems can be generated and solved by symbolic manipulation packages. For high orders the approach to the construction of such methods is based on the computation of the coefficients of the stability function by a variant of the Fourier series method and then solving the resulting large systems of polynomial equations of high degree by least squares minimization. Using these approaches both explicit and implicit methods were constructed up to the order eight with good stability properties (Runge-Kutta stability for explicit methods, A-stability and L-stability for implicit methods).

In the second part of this talk we will address different issues related to the implementation of general linear methods. They include selection of initial stepsize and starting values, computation of Nordsieck representation, efficient and reliable estimation of the local discretization errors for nonstiff and stiff equations, step size ond order changing strategies, construction of continuous interpolants, and updating vector of external approximations to the solution. Experiments with variable step variable order experimental Matlab codes for both nonstiff and stiff differential systems on interesting test problems will be presented and compared with appropriate codes from Matlab ODE suite. These experiments demonstrate the high potential of diagonally implicit multistage integration methods, especially for stiff systems of differential equations.

Equation-Free Multiscale Computation: Enabling Microscopic Simulators to Perform System Level Tasks

by

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Abstract

I will present and discuss a framework for computer-aided multiscale analysis, which enables models at a "fine" (microscopic/stochastic) level of description to perform modeling tasks at a "coarse" (macroscopic, systems) level. These macroscopic modeling tasks, yielding information over long time and large space scales, are accomplished through appropriately initialized calls to the microscopic simulator for only short times and small spatial domains: "patches" in macroscopic phase space-time.

Traditional modeling approaches start by deriving macroscopic evolution equations (balances closed through constitutive relations). An arsenal of analytical and numerical techniques for the efficient solution of such evolution equations (usually Partial Differential Equations, PDEs) is then brought to bear on the problem. Our equation-free (EF) approach, introduced in PNAS (2000) when successful, can bypass the derivation of the macroscopic evolution equations it when these equations conceptually exist but are not available in closed form.

We discuss how the mathematics-assisted development of a computational superstructure may enable alternative descriptions of the problem physics (e.g. Lattice Boltzmann (LB), Brownian Dynamics (BD), kinetic Monte Carlo (KMC) or Molecular Dynamics (MD) microscopic simulators, executed over relatively short time and space scales) to perform systems level tasks (integration over relatively large time and space scales, "coarse" bifurcation analysis, but also optimization and control tasks) directly.

In effect, the procedure constitutes a systems identification based, "closure on demand" computational toolkit, bridging microscopic/stochastic simulation with traditional continuum scientific computation and numerical analysis. We illustrate these "numerical enabling technology" ideas through examples from chemical kinetics (LB, KMC), rheology (Brownian Dynamics), homogenization and the computation of "coarsely self-similar" solutions, and discuss various features, limitations and potential extensions of the approach.

Jacobian-Free Newton-Krylov methods for the accurate time integration of stiff wave problems.

by

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Abstract

We present results from our research on using JFNK methods for the implicitly balanced time integration of stiff wave problems. We draw our examples from the areas of geophysical fluid dynamics and magnetohydrodynamics. Stiff wave problems are a classical multiple time scale problem where the fast time scale (stiff wave) physics is in a "near balance" with other normal modes in the system resulting in a slow dynamical time scale. In this situation one would like to use time steps on the order of the dynamical scale for time integration. Historically, Semi-Implicit (SI) methods have been developed to step over the stiff wave time scale in a stable fashion. However, SI methods require some linearization and time splitting, and both of these can produce additional time integration errors. Our algorithmic approach employs SI methods as preconditioners to JFNK, resulting in an implicitly balanced method (no linearization or time splitting). In this presentation we will provide an overview of SI methods in a variety of applications. We will present details of our algorithmic approach. Then we will compare accuracy and efficiency of our method with more traditional SI methods.

Time-integration of low Mach number reacting flow with detailed chemical kinetics

by

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Abstract

The time-integration of low Mach number reacting flow with detailed kinetics presents a number of challenges. Even laboratory-scale realizations of these flows with simple fuels are characterized by large ranges of length and time scales as well as significant complexity in chemical source term evaluations. Efficient time integration of these systems requires attention to be paid to both spatial and temporal discretization constructions. In this talk I will present our experiences in this field, outlining primarily time integration issues, involving projection-scheme integration of multidimensional low Mach number flames, the coupling of momentum and species time integration procedures, as well as the utility of semi-implicit (IMEX) and operator-split time-integration constructions. Given the significant costs associated with the time integration of chemical source terms, I will also discuss this area specifically, and will address various means of model reduction and/or solution-tabulation to reduce overall time integration costs.

Implicit-explicit Runge-Kutta schemes and applications to hyperbolic systems with relaxation

by

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Abstract

We present implicit-explicit (IMEX) Runge Kutta methods for hyperbolic systems of conservation laws with stiff relaxation terms. Here we restrict our analysis to diagonally implicit Runge Kutta (DIRK) schemes and consider schemes up to order 3 that are asymptotic preserving (AP) and strong-stability-preserving (SSP) in the zero relaxation limit. Accuracy and stability properties of these schemes are studied both analytically and numerically. The schemes are then combined with a weighted essentially non oscillatory (WENO) finite difference strategy in space to obtain fully discrete high order schemes. Several applications to hyperbolic relaxation systems in stiff and non stiff regimes show the efficiency and the robustness of the present approach.

Error Estimation and Control for ODEs

by

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Abstract

This talk is about the numerical solution of initial value problems for systems of ordinary differential equations (ODEs). At first these problems were solved with a fixed method and constant step size, but nowadays the general-purpose codes vary the step size, and possibly the method, as the integration proceeds. Estimating and controlling some measure of error by variation of step size/method inspires some confidence in the numerical solution and it makes possible the solution of hard problems. Common ways of doing this are explained briefly in the talk.

The NCAR Spectral Element Climate Dynamical Core: Semi-Implicit, Semi-Lagrangian Formulation

by

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Abstract

We describe the implementation of a new dynamical core for atmospheric general circulation models. To avoid singularities at the poles, a cubed-sphere coordinate system is employed. A high-order spectral element discretisation in the horizontal direction is combined with a second order finite difference scheme in the vertical. Large time steps beyond the advective CFL limit are made possible by the operator-integration factor (OIF) scheme of Maday et al (1990). A three-time level leapfrog scheme for advection is combined with a Crank-Nicholson (semi-implicit) scheme applied to the terms responsible for gravity waves. Linear stability analysis reveals that the resulting discretized system of PDE's is neutrally stable for the meteorologically important Rossby waves. Variable resolution has been implemented recently using non-conforming spectral elements with interpolation at element boundaries. Numerical results are reported for the baroclinic instability test problem proposed by Polvani et al (2003).

On Solving Highly Stiff Diffusion-Reaction Systems

by

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Abstract

For solving highly stiff diffusion-reaction systems one often adopts the implicit method of lines approach. The main issue then is how to solve the arising systems of linear and nonlinear algebraic equations. In higher space dimension this can be costly and problematical. In this talk we avoid this and adopt the explicit method of lines approach and focus on stabilized methods from the Runge-Kutta-Chebyshev family. An implicit-explicit (IMEX) extension of an existing explicit Runge-Kutta-Chebyshev (RKC) scheme designed for parabolic PDEs is proposed for diffusion-reaction problems with severely stiff reaction terms. The IMEX scheme treats these reaction terms implicitly and diffusion terms explicitly. Within the setting of linear stability theory, the new IMEX scheme is unconditionally stable for reaction terms having a Jacobian matrix with a real spectrum. For diffusion terms the stability characteristics remain unchanged. A numerical comparison for a highly stiff, nonlinear radiation-diffusion problem between an RKC solver, an IMEX-RKC solver, and the implicit BDF solver VODPK using the Krylov solver GMRES illustrates the excellent performance of the new IMEX scheme.