MATHEMATISCHES FORSCHUNGSINSTITUT OBERWOLFACH

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(letzter Bericht 1989)

Theory and Numerical Methods for Initial-Boundary Value Problems

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The conference was organized by H.O. Kreiss (UCLA, Los Angeles) and J. Lorenz (Caltech, Pasadena). It was centered around the theory and numerical treatment of time-dependent partial differential equations. A aim of the conference was to bring together practical and theoretical aspects. Once more has this conference shown that theoretical studies are of great significance for the numerical treatment and the interpretation of results.

G. Bader:

Collocation Methods for a Class of higher Index DAE's

Most present methods for the solution of DAEs require the solution of ill-conditioned (non-) linear systems of equations. As a consequence the numerical solution is polluted by round off errors. This leads to serve problems when dealing with step size controls for these discretizations. The talk presents a class of new collocation discretizations which do not suffer from round off error influence.

Greg Baker:

Flow of Fluids with Free Surfaces or Vortex Sheets

A natural description for the motion of a free-surface in an inviscid, incompressible fluid is given by a boundary integral involving a distribution of dipols (equivalent to a vortex sheet). The motion of the free-surface requires only the evaluation of the boundary integral. Numerical studies have been made of the classical Rayleigh-Taylor instability, the breaking of water waves over a bottom topography, the generation of wave-trains by submerged bodies and the rise of bouyant bubbles. However, there are circumstances when curvature singularities develop on the free-surface due to the presence of the Kelvin-Helmholtz instability. Recently, attempts have been made to understand the formation of this singularity and what the nature of the free-surface might be beyond the singularity time by employing various regularizations of the equations.

Wolf-Jürgen Beyn:

Heteroclinic and Homoclinic Orbits

Global changes in the asymptotic regime of parametrized dynamical systems often occur at separatrices. These separatrices consist of orbits connecting two unstable steady states. The talk provides some answers to the following basic questions in the theory and numerical analysis of these connecting orbits (homoclinic or heteroclinic).

- What is a well posed problem for a connecting orbit and its associate parameter set ?
- When does a branch of periodic orbits bifurcate from a homoclinic orbit ?
- If we truncate the infinite boundary value problem to a finite interval, can we choose this interval and the finite boundary conditions in an adaptive and efficient way ? What is the approximation error involved ?

Evangelos A. Coutsias:

A Spectral Algorithm for the Navier-Stokes Equations in 2D Bounded Geometries

In two dimensions, calculations of the Navier-Stokes equations are considerably simplified in the vorticity-stream function (VSF) formulation: there is only one component of the vorticity field to advance in time as opposed to two for the velocity, and the pressure calculations is replaced be the conceptionally simpler calculations of the stream function via solution of Poission's equation. Also incompressibility is automatically satisfied, while in the velocity-pressure formulation it must be enforced separately. However the no-slip condition is given on the velocity and its inclusion in the VSF formulation has been a source of difficulties. We have developed a scheme for efficient computations of the NS-VSF equations in annulus or a slab in 2d. The quantities are expanded in a Chebyshev-Fourier series. The NS equations is solved implicitly for the viscous term, while the inertial term is computed in point space and the result is dealiased using a 2/3 truncation. The resulting diffusion problem and the Poisson equation for the stream function are reduced via Chebyshev recursion to banded form and solved directly. The no-slip condition is expressed by integral constraints on the vorticity which are included as tau conditions. The algorithm is used to study the Kelvin- Helmholtz instability in linear an circular shear lows in a guiding center plasma.

Bernd Einfeldt:

On Design-Criteria for Numerical Methods for Hyperbolic Conservation Laws

In the last ten years there has been a considerable development of difference methods for nonlinear hyperbolic conservation laws. Still an open problem is the specification of design criteria in multiple space dimensions, which guarantee numerical results without spurious oscillations. The major criterion in one space dimension is that the scheme be

Total Variation Diminishing (TVD). Several second order accurate TVD schemes exists in one space dimension. But second order accurate TVD schemes do not exists in two space dimensions, at least if we use the obvious extension of this stability criterion to two space dimensions. It has been shown in [1] that a two dimensional TVD scheme is at most first order acurate. Furthermore the TVD property has not been shown for some state-of-the-art schemes as e.g. the PPM-scheme [2]. In [3] I introduced a new class of schemes (denoted as Positive schemes) which satisfy a minimum-maximum principle and it was proved that some well known schemes, for which so far no nonlinear stability results exist belong to the class of Positive schemes, this includes the PPM scheme and dimensional-splitting schemes. Further developments are reported in [4]
Starting with some remarks concerning classical design-criteria and TVD schemes we consider next the class of Positive schemes and show that a minimum-maximum principle is a appropriate criterion for the construction of oscillation-free numerical methods in one and multiple space dimensions.

1. J. Goodman and R. Leveque, "On the accuracy of stable schemes for 2D scalar conservation laws", Math. Compt. 45 (1985), pp. 15-21.
2. P. Colella and P.R. Woodward, "The piecewise parabolic method (PPM) for gas dynamical simulations", J. Compt. Phys. 54 (1984), pp. 174-201.
3. B. Einfeldt, "On Positive shock capturing schemes", College of Aeronautics Reprint No. 8810, August 1988.
4. B. Einfeldt, "Conception for the design of difference methods for nonlinear conservation laws: I. The geometric approach on regular grids.", Preprint SC 89-11 of the Konrad-Zuse-Zentrum für Informationstechnik, Berlin.

Bengt Fornberg:

An Improved Pseudospectral Method for Initial-Boundary Value Problems

Pseudospectral methods based on Jacobi-polynomials (with Chebyshev polynomials an important special case), are commonly used to obtain accurate solutions to initial-boundary value problems. With derivatives of more than first order in space, stability conditions for explicit time stepping methods become very restrictive (in case of second derivatives, they typically take the form $\Delta t = O(1/N^4)$, where N is the number of nodes). We introduce a new procedure for incorporating boundary conditions, which relaxes the constants in such conditions by an order of magnitude or more.

Moshe Goldberg:

Simple Stability Criteria for Difference Approximations to Hyperbolic Initial-Boundary Value Problems

Consider the first order system of hyperbolic equations

$$u_t(x,t) = Au_x(x,t) + Bu(x,t) + f(x,t), \qquad x \geq 0, \quad t \geq 0,$$

where $u(x,t)$ is the unknown vector, $A = diag(A^I, A^{II})$ a diagonal matrix with $A_1 > 0$ and $A_2 < 0$, B an arbitrary matrix, and $f(x,t)$ a given vector. The problem is well posed in $L_2(0,\infty)$ if initial values

$$u(x,t) = g(x) \epsilon L_2(0,\infty), \quad x \geq 0$$

and boundary conditions

$$u^I(0,t) = Su^{II}(0,t) + h(t), \quad t \geq 0,$$

are prescribed. Here u^I and u^{II} are the inflow and outflow parts of u corresponding to the partition of A, and S is a coupling matrix.
This talk describes recent and joint efforts with E. Tadmor in which we extend our 1987 results (Math. Compt. 48, pp. 503-520) in order to achieve convenient stability criteria for a wider class of finite difference approximations to the above initial-boundary value problem.

Jonathan Goodman:

1. Stable Vorticity Boundary Conditions

I discuss some results from Kalman Meth's thesis. A vorticity boundary condition for finite difference solution of the incompressible Navier Stokes equations is shown to be second order accurate and stable (by energy estimates). In three dimensions, the scheme uses a staggered mesh. I discuss interface conditions between finite difference and free vortex method computations. Results from hybrid computations will be presented.

2. Instability of the Unsmoothed Fourier Method

There has been some controversy about the stability of the unsmoothed Fourier method for the problem $u_t = \sin(x)u_x$. Writing the approximate solution as

$$U = \sum_{k=-M}^{M} U_k(t) \exp(ikx),$$

the evolution of the $U_k(t)$ is governed by a nearly tri-diagonal matrix. A GKS analysis shows that this evolution problem has a mild radiative instability.

Bertil Gustafsson:

Boundary Conditions for the Navier-Stokes Equations at Open Boundaries

It is well known how to construct well posed boundary condition for the Navier Stokes equations. However, for problems defined in unbounded domains, artificial boundaries must be introduced in order to make the computational domain finite, and in that case accurate data are most often missing. By analyzing certain model problems, we shall investigate under what conditions we still can expect accurate solutions. In particular, we shall show that simple extrapolation can be used for all dependent variables in the boundary layer near solid walls.

Laurence Halpern:

Artificial Boundary Conditions

It is well known that the solution of the Klein-Gordon equation in $\mathcal{R}^n$ $u^*_{tt} - \Delta u^* + \alpha^2 u^* = f(x)$, converges locally to a steady state $-\Delta v^* + \alpha^2 v^* = f(x)$ as t tends to infinity. We consider the Klein-Gordon equation in a bounded domain Ω, with a boundary condition $u_t + u_n + Bu = 0$, where B is a linear continuous coercive operator on $H^{1/2}(\Gamma)$. We prove that the solution converges exponentially to a steady state v, defined by $-\Delta v + \alpha^2 v = f(x)$ in Ω, $v_n + Bv = 0$ on Γ. Thus v can't be equal to v^*, unless B is the Dirichlet-to-Neumann operator for exterior steady problems. This study provides a boundary condition on Γ, which is "absorbing" for small times, and forces the convergence to the steady-state as times tends to infinity.
This is joint work with B. Enquist (UCLA).

Helmut Jarausch:

Solution of Semidiscrete Parabolic Differential Eqautions via Adaptive Spectral Decomposition

We consider (mildly) nonlinear parabolic equations which are treated by the method of lines. The resulting (large) ODE-system will be adaptively (partly) decoupled into a small system of at most mildly decreasing modes and the complementary (large) system of fast decaying (quasi stationary) modes. This decoupling can be used in advantage to take bigger stepsizes and to use an exponentially fitted implicit Euler method for the quasi stationary modes.

Peter Kloeden:

The Quasi-Geostrophic Equations

The Quasi-Geostrophic equations describe large-scale meterological phenomena with the dominant dynamics occurring in the horizontal directions. They involve stream function $\Psi(t, x, y, z)$ on a cylindrical space $\Omega \times (0, z^*)$ satisfying an equation of the form

$$\Psi_{xx} + \Psi_{yy} + \frac{1}{\rho}(\rho\alpha\Psi_z)_z. \tag{1}$$

where $\alpha(z)$ is the static stability profile, $\rho(z)$ the density profile and ω the vorticity. The vorticity satisfies an IVP

$$\omega_t + u\omega_x + v\omega_y = -\beta v, \tag{2a}$$

$$u = -\Psi_y \quad and \quad v = \Psi_x, \tag{2b}$$

where β is the Coriolis parameter. The appropriate boundary conditions for (1) involve the potential temperature $\theta = \psi_z$ being specified at $z = 0$ *and* $z = z^*$, or evolving there according to IVP of the form

$$\theta_t + u\theta_x + v\theta_y = 0. \tag{3}$$

Various existence and uniqueness theorems will be stated and their proofs outlined.

Peter Knabner:

Numerical Approximation of Reactive Solute Transport in Porous Media

We consider

$$\partial_t(\Theta u) + \rho_l \partial_t \Psi(u) + \rho_k \int_\Lambda \partial_t v(\lambda,.)d\lambda - div(D\Delta u - gu) = 0$$

$$\partial_t v(\lambda,.) = k_\lambda(\varphi(\lambda,u) - v(\lambda,.)), \quad \lambda \epsilon \Lambda, \quad (x,t)\epsilon\Omega \times (o,t]$$

with initial-boundary conditions for unknows u, v. This is a macroscopic model for solute transport in porous media with absorption, both in equilibrium and non-equilibrium. The typical absorption isotherms φ, Ψ are not Lipschitzian up to $u = 0 \quad (e.g.\varphi \sim u^p, 0, p, 1)$. We consider various time discretizations with special respect to $\partial_t \Psi(u)$, which determines the regularity of the problem. These are combined with finite elements in space.

H.O. Kreiss:

Convergence of the Solutions of the Compressible to the Solutions of the Incompressible Navier-Stokes Equations

In this talk we study the slightly compressible Navier-Stokes equations. We first consider the Cauchy problem, periodic in space. Under appropriate assumptions on the initial data, the solution of the compressible equations consists - to first order - of a solution of the incompressible equations plus a function which is highly oscillatory in time. We show that the highly oscillatory part (the sound waves) can be described by wave equations, at least locally in time. We also show that the bounded derivative principle is valid, i.e., the highly oscillatory part can be suppressed be initialization. Besides the Cauchy problem, we also consider an initial-boundary value problem. At the inflow boundary, the viscous term in the Navier-Stokes equations is important. We consider the case where the compressible pressure is prescribed at inflow. In general, one obtains a boundary layer in the pressure; in the velocities a boundary layer is not present to first approximation.

Stig Larsson:

A Finite Element Method for the Cahn-Hilliard Equation

The Cahn-Hilliard equation

$$(1) \qquad u_t - \Delta(-\Delta u + \phi(u)) = 0,$$

together with appropriate boundary and initial conditions and $\phi(u) = u^3 - u$, is a phenomenological model for phase separation and spinodal decomposition. The boundary conditions are such that the fourth order differential operator in (1) can be written as the square of a second order elliptic operator. Relying on this fact we introduce numerical schemes for (1), which, for the approximation of spatial variables, are based on standard finite element methods for second order elliptic problems. We discuss spatially semidiscrete schemes as well as a completely discrete scheme based on the backward Euler method. We prove optimal order error estimates for both smooth and non-smooth initial data. The fact that the corresponding discrete equations posses a Ljapunov functional is employed. Apart from being of independent interest, such error estimates have applications in the study of the long-time behavior of discrete solutions, e.g., in proving convergence of attractors.
This is a joint work with Charles Elliott, Brighton.

Mitchell Luskin:

Numerical methods for the Deformation of Crystals with Symmetry-Related Variants

We give computational results and numerical analysis from joint work with Charles Collins and David Kinderlehrer for several models for solid crystals with symmetry related (martensitic) variants. The solutions to the mathematical models are characterized by approximating sequences which have oscillations which converge weakly (in the sense of local spatial averages), but which do not converge strongly (pointwise). The oscillations given by the approximate sequences can be related to the microstructure observed in the crystal materials, and are described mathematically by the Young measure.
Our numerical experiments for two and three dimensional solids have exhibited microstructure on the scale of the grid. We will present a rigorous analysis of numerical methods for one-dimensional models to give a justification for the use of such numerical methods to model the behavior of this class of solid crystals.

K.W. Morton:

Finite Volume Petrov-Galerkin Methods
for Convection-Dominated Transport Problems

Upwind difference methods were devised for convection dominated problems: and Petrov-Galerkin methods from their finite element counterparts. There is an elegant theory for such methods which show that there are optimal spaces of test functions for any norm for which the Lax-Milgram lemma holds. It also gives an error bound for any choice of test space. Bounds for some common choices will be presented.

Finite volume methods have been developed with other objectives in mind, but can be regarded as nonconforming Petrov-Galerkin methods. Moreover they turn out to be extremely effective for convection-dominated problems. Recent numerical results and some error analysis will be presented.

Mu Mu:

Wellposedness of Initial-Boundary Value Problems
for Equations in Atmospheric Dynamics

The paper is concerned with wellposedness of initial-boundary value problems for equations in atmospheric dynamics. First, global existence of smooth solutions to initial-boundary value problems for vorticity and potential vorticity equations has been proved. These equations play important roles in atmospheric dynamics. The key idea is to consider these equations as hyperbolic-elliptic (including degenerate cases) composited ones. Second, we present some results on local existence of smooth solution of potential vorticity equation with nonlinear boundary condition. Whether or not there is a global smooth solution to this problem remains unsolved. Last, for three-dimensional balanced model, which is nonlinear hyperbolic-elliptic (also including degenerate case) composited-coupled systems, we have proved the existence of local classical solutions.

Rolf Rannacher:

Long-Time Error Estimates for Non-Dissipative Systems

Non-dissipative parabolic initial-boundary value problems may have solutions possessing certain global stability properties. Even if the structure of the problem does not allow for a proof of these properties, for a particular solution, one can take them as an assumption in order to establish long-term error estimates for a large class of discretization schemes. The proof is by an induction argument with respect to time tending to infinity. It is discussed which properties a discretization scheme should possess in order to make this argument work. As usual there are some problems with the classical Crank-Nicolson scheme.

R. Rautmann:

On Tests for Stability

For quasimonoton increasing C^1-vector functions f in $\Re^n$ (and even for more general functions) the local asymptotic stability of a critical point x^* of

$$(*) \qquad \frac{d}{dt}x = f(x)$$

can be checked by an $O(n^3)$-step calculation, if we use that a real Z-matrix is positively stable if and only if it is of monotone type. For a continuous quasimonoton increasing vector function f on $\Re^n$, the global asymptotic stability of a critical point x^* of $(*)$ follows from sufficient conditions that x^* is situated on a C^1-curve $X(s)\epsilon\Re^n$, which (in the component wise ordering of $\Re^n$) is strictly increasing form $-\infty$ to $+\infty$ and on which

$$0 < f(X(s)) \quad for \quad X(s) < x^*, \quad and \quad f(X(s)) < 0 \quad for \quad x^* < X(s)$$

holds. Then in addition x^* is the unique critical point of $(*)$ in $\Re^n$. By the well-known comparison theorems, these results also apply on weakly coupled quasimonoton increasing parabolic systems.

S. Titi:

Inertial Manifold Interpretation of the Finite Difference Method

By means of the inertial manifolds (IMs) theory on can show that the long time behavior of certain dissipative nonlinear partial differential equations can be fully described by the behavior of certain ordinary differential system - called an inertial form. Usually, one can not get this inertial form explicitly and instead one replaces it by an approximate inertial form, well motivated by the dynamics, in real computations.
Using the Kuramoto-Sivashinsky equations as an illustrative example we show that, by means of the IM theory, that dynamical system of the nodal values of the solution is

equivalent to that of the solutions themselves. In order to simulate the evolution of the nodal values we use the finite difference approximations; which in this context can be considered as an approximate inertial form. It is remarkable that in this example the number of determining nodes is proportional to the dimension of the IM. The same is true regarding the number of determining nodes.

Berichterstatter: B. Einfeldt