STIFF SOURCES AND NUMERICAL METHODS FOR CONSERVATION LAWS The American Institute of Mathematics

This is a hard–copy version of a web page available through http://www.aimath.org Input on this material is welcomed and can be sent to workshops@aimath.org Version: Fri Apr 1 09:58:28 2005

Table of Contents

A.	Participant Contributions	
	1.	Amadori, Debora
	2.	Chertock, Alina
	3.	Christoforou, Cleopatra
	4.	Despres, Bruno
	5.	Filbet, Francis
	6.	Gamba, Irene
	7.	Gelb, Anne
	8.	Gerritsen, Margot
	9.	Hauck, Cory
	10.	Jin, Shi
	11.	Katsaounis, Theodoros
	12.	Kroener, Dietmar
	13.	Kurganov, Alexander
	14.	Levy, Doron
	15.	Liao, Xiaomei
	16.	Lukacova, Maria
	17.	Noelle, Sebastian
	18.	Perthame, Benoit
	19.	Puppo, Gabriella
	20.	Simeoni, Chiara
	21.	Tadmor, Eitan
	22.	Xing, Yulong
	23.	Younis, Rami
	24.	Zeitlin, Vladimir

A.1 Amadori, Debora

I would be interested in the numerical approximation of the scalar equation

$$u_t + f(u)_x = \frac{1}{\varepsilon} h\left(\frac{x}{\varepsilon}\right) \tag{1}$$

with h continuous and 1-periodic, with zero average; $f \in C^1(\mathbf{R})$, $u \cdot f'(u) > 0$, $f(u) \to +\infty$ as $|u| \to +\infty$, and with 1-periodic initial data.

I can contribute some recent results on the pointwise behavior of the oscillation, as $\varepsilon \to 0$, of the solutions to (1); this analysis could be of help in the numerical approximation of (1).

More generally, I am interested in the analysis of problems that exibit resonant phenomena.

A.2 Chertock, Alina

One of the projects I am working on is aimed at developing a hybrid finite-volume-particle method for systems of conservation or balance laws coupled with a nonlinear transport equation. Solutions of such systems are usually nonsmooth: they may contain shocks, rarefaction waves and contact discontinuities. The presence of a stiff source term adds another level of complexity to the model. Such problems arise, for instance, in modeling transport of a passive pollutant in shallow water (in which case the source of the pollutant may be even a point-source modeled by a delta-function) or compressible inviscid reacting gases (in which case the source is usually stiff, since the reaction is fast and the time scale associated with the reaction is much smaller than that associated with the fluid advection). It is well known that numerical dissipation present in shock-capturing methods may not only seriously degrade the quality of the computed solution but may also lead to nonphysical states, which in turn, may completely destroy the numerical solution.

The core idea of the new method is to use a finite-volume method to numerically integrate a system of conservation (balance) laws and a particle method to solve transport equations coupled with the system. This way the specific advantages of each scheme are utilized at the right place. Particle methods applied to transport equations, can ameliorate most of the problems posed by the presence of numerical viscosity since particles provide a non-dissipative approximation of the convection. In these methods, the solution is sought in the form of a linear combination of the delta-functions, whose positions and coefficients represent locations and weights of the particles, respectively. The locations and weights of the particles are then evolved in time according to a system of ODEs, obtained from the weak formulation of the transport equations.

We have successfully implemented the finite-volume-particle method for the above as well as some other (inviscid) models and we plan to apply the method to more realistic advection-diffusion-reaction models. This extension is not straightforward since it will involve the treatment of diffusion and reaction terms that may appear in the equation. There was a number of attempts in the past to use particle methods for approximating solutions of convection-diffusion models, but each of them has its own drawback, associated primarily with the reconstruction of the point values of the computed solution from its particle distribution. Most of known recovering procedures, suitable for smooth functions, typically fail

to produce reasonable results in the nonsmooth case. In the purely convective case, we were able to overcome this difficulty using the concept of the dual equation, but it is not clear whether this approach can be generalized for the viscous case.

Another (theoretical) difficulty one may encounter while implementing the finite-volume-particle method is related to the lack of smoothness in the right-hand side of the ODE system that describes the evolution of particles and their weights. While the existence of a generalized solution is guaranteed by the theory of Filippov, the uniqueness can only be obtained via a proper regularization. The presence of a point-source term makes the problem even more challenging and a theoretical justification of the particle method in this case is a wide open problem.

A.3 Christoforou, Cleopatra

My area of interest is the theory of hyperbolic conservation laws. My current research is an application of the method of vanishing viscosity: The aim is to construct solutions of hyperbolic systems of balance laws with dissipative source terms

$$u_t + (f(u))_x + g(u) = 0$$

as limits of solutions of parabolic systems

$$u_t^{\epsilon} + (f(u^{\epsilon}))_x + g(u^{\epsilon}) = \epsilon u_{rr}^{\epsilon}$$

with viscosity ϵ tending to zero. The analysis of the vanishing viscosity method of Bianchini and Bressan [BiB] is extended to this class of systems. Because of the presence of the dissipative source terms, supplementary Lyapunov functionals are constructed and additional techniques are employed to those already devised in [BiB]. Moreover, an exponential decay of the total variation of vanishing viscosity approximations is established. I am interested in applying these techniques to other systems of conservation laws. A very challenging question would be the case of systems with physical viscosity.

Finally, I am very interested in increasing my knowledge in mathematical biology. It is a challenging, fast-growing area that together with numerical methods will introduce me to new tools and assist me to improve my ability to work with physical problems.

A.4 Despres, Bruno

My interests go in two directions.

The first one is not directly related to the subject of the Workshop. It is about the theory of convergence of Finite Volume schemes by means of the old consistency+stability-implies-convergence approach. It helps to get a linear approach of the convegrence of these methods and it is possible to prove quite accurate results even for a non linear scalar conservation law.

The other one is directly related to the subject of Workshop. With a colleague (Christophe Buet) we are currently working on the numerical approximation of the model problem

$$\begin{cases} u_t + \frac{1}{\varepsilon}v_x = 0, \\ v_t + \frac{\varepsilon}{\varepsilon}f(u, v) = -\frac{\sigma}{\varepsilon^2}v. \end{cases}$$

Our idea is that we absolutely need an implicite solver for time step requirements of the diffusion limit. Various stability criteria are possible. If the model is the moment modelization of some kinetic equation, then $\frac{|v|}{u} \leq 1$ is natural. We have develop a 1D solver for this

system: the solver is implicit (we only solve a linear system with ad-hoc frozen coefficients), stable $(\frac{|v|}{u} \le 1)$, and has the correct diffusion limit. I will be happy to compare this approach with others.

A.5 Filbet, Francis

Approximation of Hyperbolic Models for Chemosensitive Movement

Numerical methods with different orders of accuracy are proposed to approximate hyperbolic models for chemosensitive movements. On the one hand, first and second order well-balanced finite volume schemes are presented. This approach provides an exact conservation of the steady state solutions. On the other hand, a high order finite difference weighted essentially non-oscillatory (WENO) scheme is constructed and the well-balanced reconstruction is adapted to this scheme in order to exactly preserve steady states and to retain high order accuracy. Numerical simulations are performed to verify accuracy and the well-balanced property of the proposed schemes and to observe the formation of networks in the hyperbolic models similar to those observed in the experiments.

Keywords: chemotaxis, hyperbolic systems, finite volume methods, finite difference methods, WENO schemes, well-balanced schemes.

This work is in collaboration with Chi-Wang Shu, Brown University

A.6 Gamba, Irene

Non-equilibrium time dependent reactive kinetic-Poisson systems appear in the modeling of such diverse areas as electron transport in solids, biological transport, granular and energy dissipative flows. These non-conservative systems exhibit a common feature: their steady or self similar states are given by statistical Stationary Non-equilibrium States (SNS), meaning they are far deviated from Gaussian probability distributions. They entice approximating hydrodynamic models modeling "source" representing momentum and energy gain or dissipation due to strong friction or forcing scales.

When these non-equilibrium regimes take over, classical hydrodynamic models (based on Gaussians/Maxwellian closures) do not apply and need to be corrected to account for the non-equilibrium statistics.

I am interested in issues related to the mathematical properties of these models such as existence, uniqueness, self-similarity, stability and to analyze their higher order moment equations (hydro-dynamical corrections) and corresponding boundary value problems; as well as to investigate optimal numerical simulation methods for corresponding quantum, kinetic and macroscopic (hydrodynamic) models.

I will present a very recent work related to item (1.i) below:

"Deterministic solvers to transient Boltzmann-Poisson equations"

Abstract: The Boltzmann-Poisson system is the most reliable model for the flow of charged particles in semiconductors devices. Real device models have not already been simulated by deterministic computations due to its high computational cost, although is very well known and general practice to solve these models by Monte-Carlo (DSMC) methods.

We focus in a rather easy and fast deterministic solver for a channel flow: one and two-dimension and three-velocity dimension. The system of equations reduces to a linear kinetic (non-local) equation solved by WENO methods coupled with the Poisson equation for the force field acting on the particles accounting for long range interactions. We will focus on the development of the method, simulation results for diodes and MESFET as well as comparisons to other classical models in the field. In particular we compute, deterministically, the evolution probability density function with its first three moments. Boundary singularities for 2-space dimensions models are accurately computed.

This work has been done in collaboration with J.A. Carrillo, A. Majorana and C.-W. Shu.

Finally, I will present work in progress on computations by DG schemes of linear Boltzmann equations, work in collaboration with Jennifer Proft and Ross Heath.

Some other issues I am and have been studying, and I am interested in learning more, are:

- 1)Self-consistent models of kinetic charged transport. Perturbations of Stationary Non-Equilibrium States (SNS).
- 1.i) Numerical implementation of deterministic kinetic-Poisson systems and comparisons to DSMC simulations by WENO schemes, and more recently, developing Discontinuous Galerkin (DG) schemes.
- 1.ii)Boundary value problems, existence and hydrodynamics limits for strong force fields. Coupling of hyperbolic (SNS) and diffusion (SES) scaling regimes by kinetic layers.
 - 1.iii)Biological transport of charged molecules and Chemotaxis kinetic transport.
- 2) Quantum Trajectory Models (QTM) for charged transport and Quantum hydrodynamics (QHD) from a semi-classical picture: thermalization and Bose-Einstein condensates models. Existence and non-existence to dispersion/diffusion models. Applications and computations.
- 2.i) Strong force field (Chapman-Enskog) expansion to the semi-classical Wigner transport equation
 - 2.ii) Finite time flow up for the QHD equations under high velocity data
 - 2.iii) Numerical calculations for quantum states.
- 3) The Boltzmann equation for energy dissipative flows, such as inelastic collisions in the modeling of rapid granular flows or elastic collisions in mixtures.
- 3.i) Energy dissipative Maxwell model type-solutions with power like tails-Levy distributions. Trends to equilibrium for energy dissipative Pseudo Maxwell models.
- 3.ii) Point-wise upper bounds for variable hard spheres, both in the elastic and inelastic case. Boundary value problems. Space inhomogeneous equation.
 - 3.iii) Numerical implementations by spectral methods

References can be found at www.ma.utexas.edu/users/gamba/research.html

A.7 Gelb, Anne

I am most interested in shallow water equations as they pertain to environmental fluid dynamics. Specifically I am interested in global and local methods as they can be applied to spheres. I am also interested in problems of long term simulations.

A.8 Gerritsen, Margot

Joint contribution with Rami Younis.

Our general area of interest is the efficient numerical solution of flow and transport equations in reservoirs. At the moment, we focus primarily on the design of accurate methods for simulation of miscible gas injection and in-situ combustion (or fire-flooding), which

are important Enhanced Oil Recovery processes. These processes are inherently multi-scale. They are generally modeled by two sets of equations. One describing the general flow and energy (if non isothermal) in the reservoir, which either parabolic in character. The second set models transport of components present in the oil, gas and water in the reservoir. The resulting equations are (weakly) hyperbolic, and very strongly nonlinear. In in-situ combustion processes additional reaction terms render the system also very stiff. We are exploring Euler-Lagrangian type methods for gas injection processes, and splitting techniques for treatment of the equations governing in-situ combustion.

A.9 Hauck, Cory

My interest in this workshop stems from work on hydrodynamic models of electron transport in semiconductors. These models are balance laws that approximate the evolution of a kinetic distribution of electrons by tracking a given set of velocity and/or energy moments. Hydrodynamic equations contain conservative terms, relaxation terms that arise from collisions, and drift terms derived from a electrical potential that satisfies a Poisson equation.

Hydrodynamic equations suffer from several difficulties. First of all, most electronic devices contain some type of abrupt material interface which make it difficult to devise a numerical scheme that properly captures the balance of forces found at the differential level. For high-field, transition-regime devices, numerical results are characterized by current oscillations that pollute the solution and can even cause breakdown via negative temperatures and densities. It would very helpful to know if this issue can be overcome with a well-balanced numerical scheme or whether it is a model defect.

Second, in the low-field, high-density limit, the hydrodynamic equations recover the well-known drift-diffusion model. Hydrodynamic equations become stiff in this limit, and this includes stiff flux terms. Thus, with the restrictions given by a CFL condition, it is not straightforward how to implement an implicit scheme in an efficient way.

Finally, I am interested in finding reasonable approximations to relaxation terms and, in particular, relaxation times. In gas dynamics there is an issue of obtaining the correct transport coefficients predicted by the kinetic model in the fluid limit. More specifically, one would like to recover an appropriate ratio of thermal conductivity to viscosity. In electron transport, the drift-diffusion equations contain only one transport coefficient — the mobility — and therefore this is not an issue. However, the behavior of a numerical solution, especially the current and the temperature, is still drastically affecting by the choice of transport coefficients. Although this is more of a physical modeling issue, I think it is important to understand the effects of relaxation times on numerical solutions.

A.10 Jin, Shi

My recent interests include numerical methods for physical problems involving multiple scales. In particular I am interested in the transition from quantum to classical mechanics, from kinetic theory to hydrodynamics, and its numerical relavance. In the workshop I will present recent results on numerical methods for Liouville equations with singular Hamiltonians (which arise either from a discontinuous potential or a discontinuous local wave speed).

A.11 Katsaounis, Theodoros

Balance laws appear as mathematical models in a great number of applications areas such as gas dynamics, mechanics, geophysics, biology. In recent years there has been enormous activity on developing numerical methods for capturing correctly the properties and features of the analytical solutions. I am particularly interested in developing numerical schemes for balance laws using relaxation approximation.

The starting point of our approach is the class of relaxation schemes, introduced in [JX], which are based on the relaxation approximation to the nonlinear conservation law, that has a linear convection term and needs neither a Riemann solver nor the characteristic decomposition and thus enjoys great simplicity in the expense of increasing the number of unknowns. The stabilization mechanisms are the regularization by wave operators. The idea is to use a local relaxation approximation to construct linear hyperbolic system with a stiff lower order term that approximates the original nonlinear system with a small dissipative correction. Relaxation is a flux approximation and relaxation linearizes the Riemann problem. This simplicity can be of great significance when one has to solve large-scale engineering problems.

The numerical schemes are based on finite volume and finite element discretizations of the relaxation models. In [DK1], [DK2] the finite volume(difference) method is used to descritize the relaxation approximation of the shallow water equations in one and two space dimensions respectively. The source term is treated in two different ways. The numerical schemes are of first or second order in space and time, do not need Riemann solvers, they are able to treat the dry bed case(vacuum case) with no extra effort, and satisfy the steady states, an important feature of the analytical solution, within the accuracy of the relaxation parameter ϵ .

In [DK3] the numerical schemes presented in [DK1], [DK2] are used to compute the transport and diffusion of a passive pollutant by a water flow. The flow is modeled by the well-known shallow water equations and the pollutant propagation is described by a transport equation. It's worth mentioning that that no special treatment is needed for the transport equation in order to obtain accurate results.

The relaxation approximation of conservation laws provide a natural setting for applying the finite element method. We apply the standard finite element method combined with appropriate Runge-Kutta methods for the time discretization. Adaptive mesh refinement strategies based on a-posteriori indicators and inverse inequalities are employed for resolving accurately regions with shocks. The resulting schemes have a regularization mechanism with finite speed of propagation, do not need the solution of approximate local Riemann problems, can be formulated as low order or high order schemes, or even a combination of them (h-p methods), and can be extended in multi-dimensions by using the finite element framework, [AKM], [KM], [GM]. Some properties of these schemes, concerning stability and convergence are presented in [AMT].

Simulating a shear band (a narrow layer of intense shearing in a material, not a crack though) is another topic of interest. The mathematical model consists of a system of conservation laws, close related to that of elastodynamics. The highly nonlinear model has a internal diffusion mechanism which collapses on the shear band. The temperature and the strain rate grow (blow up?) while the velocity develops a δ -function behavior. It is an open question whether the temperature and the strain rate blow up in finite or infinite time. Numerical simulation of this singular behavior is a challenge, [BKT].

Bibliography

[AKM] Ch. Arvanitis, Th. Katsaounis, Ch.Makridakis, Adaptive Finite Element Relaxation Schemes for Hyperbolic Conservation Laws, Mathematical Modelling and Numerical Analysis, (M2AN), vol. 35, no 1, pp.17-34, 2001,

[AMT] Ch. Arvanitis, Ch.Makridakis, T. Tzavaras, Stability and convergence of a class of finite element schemes for hyperbolic systems of conservation laws, SIAM J. of Numerical Analysis, Vol. 42, No. 4, pp. 1357-1393, 2004

[BKT] Th. Baxevanis, Th. Katsaounis, A. Tzavaras, A finite element method computing shear band formation, Hyperbolic Problems: Theory, Numerics, Applications (Proceedings HYP2004),

[DK1] A. I. Delis and Th. Katsaounis, Relaxation schemes for the shallow water equations Int. J. Numer. Meth.Fluids, 41 (2003), pp. 695-719

[DK2] A. I. Delis and Th. Katsaounis, Numerical solution of the two dimensional shallow water equations by the application of relaxation methods, to appear in Applied Mathematical Modeling

[DK3] A. I. Delis and Th. Katsaounis, A generalized relaxation method for transport and diffusion of pollutant models in shallow water, Computational Methods in Applied Mathematics, vol. 4, no. 4, pp.410-430, 2004

[KM] Th. Katsaounis, Ch.Makridakis, Relaxation models and finite element schemes for the shallow water equation, Hyperbolic Problems: Theory, Numerics, Applications, T.Hou, E.Tadmor Eds, (Proceedings HYP2002), pp.621-631, Springer Verlag 2003

[GM] L. Gosse, Ch. Makridakis, Two a posteriori error estimates for one dimensional scalar conservation laws. SIAM J. Numer. Anal. 38 (2000) 964-988.

[JX] S. Jin and Z. Xin, The relaxing schemes of conservations laws in arbitrary space dimensions Comm. Pure Appl. Math., 48 (1995), pp. 235-277.

A.12 Kroener, Dietmar

My main research topics concern the analysis of numerical schemes for convection dominated flows, in particular convergence analysis, adaptive grid refinement, a posteriori error estimates, discontinuous Galerkin schemes and discretisations for problems with source terms. Applications include the MHD-, the compressible Euler- and Navier-Stokes-equations as well as the system for flow through porous media.

A.13 Kurganov, Alexander

I have been recently working on the development of numerical methods for hyperbolic systems of balance laws. One of the key examples is the Saint Venant system of shallow water equations with the source term due to the bottom topography. Besides accurately capturing shocks, contact discontinuities, and rarefaction waves, it is very important for the scheme to be able preserve both the positivity of the water height and the discrete balance between the fluxes and the source. There are several high-order methods that satisfy all these requirements, but some of the problems are still very challenging. For example, the cases when the bottom is modeled by the discontinuous function or/and when there are some

regions that get dry only for some finite time intervals and then get filled back by the water are of particular interest.

The system gets even more interesting when a transport equation describing the propagation of pollutant is added, especially when the source of pollutant is not turned off (the source is sometimes a point-source modeled by the delta-function). When the pollutant is passive, we have successfully used a deterministic particle method for its tracing, while the Saint Venant system has been solved by the central-upwind finite-volume scheme (this results in a hybrid finite-volume-particle method). However, if the pollutant is diffusing and/or reacting, then the extension of the finite-volume-particle method is not so obvious and the task of accurately tracing the pollutant becomes much more challenging.

Another extension of the Saint Venant system is the multilayer shallow water equations. They are significantly more complicated due to the nonconservative terms used to model the momentum exchange between the layers. A quality of the numerical method would obviously depend on the way the nonconservative products are discretized. We believe that, as in the single layer case, the key point is ability of the scheme to preserve (stationary) steady states and positivity of the width of each layer, but a lack of rigorous mathematical formulation/justification of the model makes it hard to design reliable numerical methods.

A similar problem arises in designing numerical methods for multiphase models, in which the governing equations are obtained by averaging over a large number of material interfaces without tracking any of them individually (this needs to be done, for example, in modeling bubbly liquids, when capturing the propagation of each bubble is simply unrealistic). The momentum and energy exchange terms are nonconservative and their discretization is even more challenging than in the multilayer shallow water case. Additional difficulty is related to the presence of stiff pressure and velocity relaxation terms.

A.14 Levy, Doron

My personal experience is dealing with balance laws follows from a series of works. Two of these works deal with the shallow water equations with bottom topography. In both works we extended central schemes for conservation laws to balance laws. First, together with Kurganov, we derived a central scheme on Cartesian meshes that satisfies the "lake in rest" constraint, preserves the positivity of the solution, and handles dry states [3]. Recently, Steve Bryson and I have extended this scheme to unstructured meshes (preserving stationary steady-state solutions) [2].

In some sense, from a numerical point of view, we have realized that the challenge always boils down to the question as of how to discretize the source terms, in such a way that the constraints are satisfied. I have been dealing with related questions in some other recent works:

- 1) modeling the dynamics of the solar atmosphere (together with Bryson and Kosovichev) [1]. Here some of the challenges were in numerically maintaining initial hydrostatic balance.
- 2) stable schemes for the incompressible Euler and Navier-Stokes equations [4]. Some connections to related issues are made over there.

There are several goals I hope to obtain in this meeting:

1) A discussion on the models. Balance laws with (and without) stiff source terms exist in many applications. My experience shows that engineers are not always interested in the

equations that mathematicians are trying to solve. Several questions follow: are we solving the right problems? what problems should be look at?

- 2) Regarding specific models: e.g., the shallow water equations with bottom topography, a problem that a lot of the conference participants seem to be interested in. What are the open problems? For example, with these specific equations, what can't we solve? (and why?) Similar questions hold for other models as well.
- 3) Numerical methods: a lot of work has been put into developing numerical methods for balance laws in recent years. It will be interesting to survey some of the recent results and successes and even more importantly to try to explicitly define what kind of problems we still do not know how to deal with numerically. Then try to understand why.
- [1] S. Bryson, A. Kosovichev, and D. Levy, High-Order Shock Capturing Methods for Modelling Dynamics of the Solar Atmosphere, Physica D., 201 (2005), pp.1–26.
- [2] S. Bryson and D. Levy, Balanced Central Schemes for the Shallow Water Equations on Unstructured Grids, SIAM Journal on Scientific Computing, accepted.
- [3] A. Kurganov and D. Levy, Central-Upwind Schemes for the Saint-Venant System With a Source Term, Mathematical Modelling and Numerical Analysis, 36 (2002), pp.397-425.
- [4] D. Levy, A Stable Semi-Discrete Central Scheme for the Two-Dimensional Incompressible Euler Equations, IMA Journal of Numerical Analysis, accepted.

A.15 Liao, Xiaomei

There are two different descriptions for the motion of an ensemble of particles under the influence of internal and external forces. One is via the viewpoint of classical trajectories, the other one is via quantum mechanical wave functions. The corresponding two models are the classical Vlasov-Poisson equation and the quantum mechanical Schrödinger-Poisson equation. It's important to relate these two descriptions since transport processes in semi-conductors are often studied in regimes on the border between the classical and quantum mechanical view of the world. This relation is well described by vanishing Planck constant $\epsilon \to 0$ in Schrödinger equations, which means the transition from quantum mechanics to classical mechanics and deserves the name "semi-classical limit". Some special interest is in the semi-classical limit of the Schrödinger-Poisson system, which is frequently used in the study of quantum transport and quantum semiconductor modelling.

The semi-classical limit of Schrödinger-Poisson in one dimensional space is pretty closed to be well understood now. But it's still open in higher dimensional space, especially after singularity. It's also interesting to do the numerical simulation to check this semi-classical limit if there is some difficulty in theory now. The related numerical simulation includes the schemes for Vlasov-Poisson equation and the multi-value solution of the corresponding moment system, the schemes for Euler-Poisson, etc.

A.16 Lukacova, Maria

In my recent research I have been dealing with multidimensional hyperbolic balance laws

$$u_t + \sum_{i=1}^{d} f_i(u)_{x_i} = b(u, x, y), \tag{2}$$

where u is the vector of conservative variables, f_i , i = 1, ..., d are flux functions, d denotes the dimension, and b(u, x, y) is a source term. Our aim is to derive a scheme which

- approximates correctly multidimensional wave phenomena / shocks (takes into account all infinitely many directions of wave propagations)
- preserves steady and quasi-steady states exactly or at least up to the second order of accuracy (well-balanced schemes), cf., e.g. [botta], [greenberg], [kurganov], [lv1] for other related approaches.

There are many practical applications where the balance laws and the correct approximation of their quasi-steady states are necessary. Some examples include shallow water equations with the source terms modelling the bottom topography, which arise in oceanography and river flow simulations. Shallow water equations with source terms modelling the Coriolis forces are used in climate modelling and meteorology for (quasi-) geostrophic flow, see, e.g., [botta], [klein], [klein2]. Further examples includes the gas dynamic equations with geometrical source terms, e.g. a duct with variable cross-section, or fluid dynamics with gravitational terms. In what follows we briefly illustrate our methodology on the example of the shallow water equations with the source terms modelling the bottom topography, the Coriolis forces and the friction effects. The results can be generalized to more complex systems of balance laws. The shallow water equations read

$$u_t + f_1(u)_x + f_2(u)_y = b(u), (3)$$

where

$$\mathbf{u} = \begin{pmatrix} h \\ hu \\ hv \end{pmatrix}, \ f_1(u) = \begin{pmatrix} hu \\ hu^2 + \frac{1}{2}gh^2 \\ huv \end{pmatrix}, (4)$$

$$\mathbf{f}_2(u) = \begin{pmatrix} hv \\ huv \\ hv^2 + \frac{1}{2}gh^2 \end{pmatrix}, \ b(u) = \begin{pmatrix} 0 \\ -ghb_x + fhv - ghS_{fx} \\ -ghb_y - fhu - ghS_{fy} \end{pmatrix}. (5)$$

Here h denotes the water depth, u, v are vertically averaged velocity components in x- and y- direction, g stands for the gravitational constant, f is the Coriolis parameter, and b=b(x,y) denotes the bottom topography and the friction slopes S_{fx}, S_{fy} describe the friction effects in the boundary layer between the fluid and the bottom.

Let us note that in some practical geophysical applications, especially in the river flow modelling or oceanography, the friction effects are very important. The determination of the friction slopes S_f is a very complex problem. The bottom composition of a river varies very rapidly, especially when vegetation is taken into account. In the literature several simplified models in order to determine the friction slope can be found. Basis for our calculation is the friction law of Darcy-Weisbach. Thus, the friction slopes are evaluated as

$$S_{fx} = \frac{\lambda u \sqrt{u^2 + v^2}}{8g h}, \quad S_{fy} = \frac{\lambda v \sqrt{u^2 + v^2}}{8g h},$$
 (6)

where λ stays for the so-called resistance value, which is determined according to the simplified form of the Colebrook-White relation

$$\frac{1}{\sqrt{\lambda}} = -2.03 \log \left(\frac{k_s/r_{hy}}{14.84} \right).$$

Here k_s denotes the friction parameter, which depends on the composition of the river bottom. Typically, k_s can vary from 1 mm for beton until 300 mm for bottom with dense vegetation.

In general the reliable approximation of the above hyperbolic balance laws is a challenging problem due to several difficulties. First, if the characteristic time step for the evolution of source term is much smaller than the time step of the convection part the problem is stiff. The reliable methods should be positivity preserving and need to correctly approximate dry zones, i.e. h = hu = hv = 0. As already mentioned above the steady or stationary solutions have to be preserved and the numerical method should not evolve steady or stationary solutions introducing spurious waves. Physically reliable solutions need to satisfied corresponding entropy condition. In this context it should be pointed out that the so-called resonance phenomenon can appear in the solution leading to its non-uniqueness. In the case of the shallow water equations it can happen for example under large topographical changes, when the subcritical flow changes to the supercritical one through transcritical stationary shock.

The basis of our numerical approach is the finite volume evolution Galerkin (FVEG) scheme, which belongs to the class of genuinely multidimensional finite volume schemes. The FVEG methods has been derived for homogeneous hyperbolic conservation laws by Lukáčová, Morton and Warnecke, cf. [fvca3]-[3d]. It couples a finite volume formulation with approximate evolution operators which are based on the theory of bicharacteristics for the first order systems [mathcom]. As a result exact integral equations for linear or linearized hyperbolic conservation laws can be derived, which take into account all of the infinitely many directions of wave propagation. In the finite volume framework the approximate evolution operators are used to evolve the solution along the cell interfaces up to an intermediate time level $t_{n+1/2}$ in order to compute fluxes. This step can be considered as a predictor step. In the corrector step the finite volume update is done. The FVEG schemes have been studied systematically from the theoretical as well as experimental point of view with respect to their stability and accuracy. Extensive numerical experiments confirm robustness, good multidimensional behaviour, high accuracy, stability, and efficiency of the FVEG schemes, see, e.g. [jcp], [sisc].

In our recent works [lv], [ln] we have generalized the FVEG scheme for hyperbolic balanced laws and derived the well-balanced FVEG method. First, using the theory of bicharacteristics we derive the approximate evolution operator, that includes the time evolution of the physical source terms. They need to be approximated in a suitable way, such that steady states are preserved. This is the predictor step, in which the so-called well-balanced approximate evolution operator is used in order to predict intermediate solution at cell-interfaces. It should be pointed out that this genuinely multi-dimensional predictor step is in some sense an analogy of the one-dimensional hydrostatic reconstruction due to Audusse et al. [bouchut1].

In the corrector step the well-balanced approximation of the source terms in the finite-volume update is done using the interface-based approximation of the source term, see [shi-jin]. In order to obtain the well-balanced approximation of the Coriolis forces as well as of the friction terms we evaluate their primitives approximatively. They are then use in an analogous way as the bottom topography slope in the well-balanced approximation of the source term.

In cooperation with Noelle [ln] we have proved that our well-balanced FVEG method preserves exactly stationary states (i.e. u = 0 = v and h + b = const.) as well as the steady jet in the rotational frame (i.e. $u = 0, v = v(x), b = b(x), h = h(x), \partial_x(h + b) = \frac{f}{g}v$), cf. [bouchut2]. The friction effects have not been included in these theoretical results. Extensive experimental treatment confirm that stationary states, their small perturbations as well as steady jets in the rotational frame are preserved up to the machine accuracy.

Open problem:

Consider two-dimensional shallow water equations with source terms modelling the bottom topography and Coriolis forces. Find a methodology to derive multidimensional schemes which preserve for any two-dimensional flow

- stationary states, i.e. $\partial_t h = 0, \partial_t u = 0, \partial_t v = 0$
- steady states, i.e. $g\partial_x(h+b) = fv$, $g\partial_y(h+b) = -fu$.

Bibliography

[bouchut1] Audusse E, Bouchut F, Bristeau M-O, Klein R, Perthame B. A fast and stable well-balanced scheme with hydrostatic reconstruction for shallow water flows, to appear in SIAM J. Sci. Comp. (2004)

[botta] Botta N, Klein R, Langenberg S, Lützenkirchen S. Well balanced finite volume methods for nearly hydrostatic flows. *J. Comp. Phys.* 2004; **196**: 539-565.

[bouchut2] Bouchut F, Le Sommer J, Zeitlin V. Frontal geostrophic adjustment and nonlinear-wave phenomena in one dimensional rotating shallow water. Part 2: high-resolution numerical simulations, to appear in *J. Fluid Mech.* 2004.

[greenberg] Greenberg JM, LeRoux A-Y. A well-balanced scheme for numerical processing of source terms in hyperbolic equations, SIAM J. Numer. Anal. 1996; **33**:1-16.

[klein] Klein R. An applied mathematical view of meteorological modelling, *In: Proceedings ICAM 2003*, eds. J.M.Hill and R. Moore, 2003; pp. 227-270.

[kurganov] Kurganov A, Levy D. Central-upwind schemes for the Saint-Venant system. M^2AN , Math. Model. Numer. Anal. 2002; **36(3)**:397-425.

[lv1] LeVeque RJ. Balancing source terms and flux gradients in high-resolution Godunov methods: The quasi-steady wave propagation algorithm. *J. Comp. Phys.* 1998; **146**:346-365.

[fvca3] Lukáčová-Medviová M. Multidimensional bicharacteristics finite volume methods for the shallow water equations. In: *Finite Volumes for Complex Applications*, eds. R. Hérbin and D. Kröner, Hermes, 2002, 389-397.

[mathcom] Lukáčová-Medviová M, Morton KW, Warnecke G. Evolution Galerkin methods for hyperbolic systems in two space dimensions. *MathComp.* 2000; **69**:1355–1384.

[jcp] Lukáčová-Medviová M, Saibertová J, Warnecke G. Finite volume evolution Galerkin methods for nonlinear hyperbolic systems. *J. Comp. Phys.* 2002; **183**:533-562.

[sisc] Lukáčová-Medviová M, Morton KW, Warnecke G. Finite volume evolution Galerkin (FVEG) methods for hyperbolic problems. SIAM J. Sci. Comput. 2004; **26(1)**:1-30.

[3d] Lukáčová-Medviová M, Warnecke G, Zahaykah Y. Finite volume evolution Galerkin schemes for three-dimensional wave equation system. submitted, 2004.

[ln] Lukáčová-Medviová M, Noelle S. Well-balanced finite volume evolution Galerkin methods for the shallow water equations. in preparation.

[lv] Lukáčová-Medviová M, Vlk Z. Well-balanced finite volume evolution Galerkin methods for the shallow water equations with source terms, Int. J. Numer. Fluids, 2004, accepted.

[klein2] Majda A.J, Klein R. Systematic multiscale models for tropics. *J. Atmos. Sci* 2003; **60**:393-408.

[noelle] Noelle S. The MOT-ICE: a new high-resolution wave-propagation algorithm for multi-dimensional systems of conservative laws based on Fey's method of transport. J. $Comput.\ Phys.\ 2000;\ 164:283-334.$

[shijin] Shi J. A steady-state capturing method for hyperbolic systems with geometrical source terms. M^2AN , Math. Model. Numer. Anal. 2001; **35(4)**:631-646.

A.17 Noelle, Sebastian

I/ Geophysical flows.

At the center of my recent interests are geophysical flows:

Paper with Jostein Natvig, Normann Pankratz, Gabriella Puppo

"Well-balanced finite volume schemes of arbitrary order of accuracy for shallow water flows"

Abstract:

Many geophysical flows are merely perturbations of some fundamental equilibrium state. If a numerical scheme shall capture such flows efficiently, it should be able to preserve the unperturbed equilibrium state at the discrete level. Here we present a class of schemes of any desired order of accuracy which preserve the lake at rest perfectly. These schemes should have an impact for studying important classes of lake and ocean flows.

Related issues that I would like to discuss:

I am more and more closely interacting with people from water and ocean research. I want to understand

- 1. the phenomena they are interested in.
- 2. the derivation and range of applicability of their models, e.g. shallow water vs Navier-Stokes.
 - 3. the numerical methods they use, often rather successfully.
 - 4. the possible impact of us as numerical analysts.
 - II/ Adjoint error control

Together with Christina Steiner, we are deriving an adaptive time step control for instationary aerodynamical problems using adjoint error control. Together with Roland Schaefer, I am beginning to use the method to control geophysical flows. Another issue is adaptive modelling. I would like to discuss the potential and the possible risks at the workshop, perhaps in the form of a roundtable discussion.

A.18 Perthame, Benoit

Balance laws with source terms are particularly interesting and difficult for their numerical solution. Indeed, by opposition to the 'free case', the constant states are no longer determinant in this case. Steady states are obtained by balancing the flux and the source.

As a consequence such a balancing is fundamental in the numerical solution. In the framework of Finite Volumes, this leads to 'Upwind the Source at Interfaces' rather than centering it. A particularly well studied case is that of Saint-Venant system with topography

which leads to well-balanced schemes. Interesting is to compare numerical algorithms and share the experience on how they work.

Other examples are

- -) rotating fluids in ocean/atmosphere
- -) friction terms
- -) diffusion limit for strong friction

I would be mostly interested in discussing and learning other cases of such systems with sources especially

- -) which applications lead to such modeling in general
- -) are there new difficulties arising
- -) specific problems from biology (chemotaxis?)

From the numerical side, I would be interested in notions and consistancy and stability associated to these schemes on non-uniform grids (motivated by triangles in 2D...etc)

A.19 Puppo, Gabriella

In the last year I've been working, with Giovanni Russo of the University of Catania) to the development of high accurate numerical schemes for stiff balance laws. These methods are based on IMEX time discretizations. IMEX (Implicit - Explicit) Runge-Kutta schemes allow to treat stiff balance laws with the techniques already developed for conservation laws. With these time marching schemes in fact it is possible to integrate convective terms explicitly, while using an implicit scheme for the stiff terms.

With this technique, we have developed finite difference schemes on staggered and unstaggered grids for stiff balance laws. These schemes so far have been implemented only in one dimensional problems, but several aspects deserve further investigation.

For one thing, these schemes must have an L-stable implicit part, in order to decay to the correct limit equation, when the stiffness parameter goes to infinity. This requirement causes a severe restriction, and the schemes obtained so far, to my knowledge, are only up to third order accurate. Is it possible to get higher order IMEX schemes?

Another interesting issue is that IMEX schemes are a sort of splitting methods. Is it possible to obtain IMEX schemes respecting some further requirement, as, say, the preservation of equilibrium states in shallow water equations?

The effectiveness of IMEX schemes derives also from the possibility of separating the issues of space and time discretizations. It is in fact particularly easy to implement the IMEX idea on semidiscrete schemes for conservation laws. However, in this fashion, one inherits all the weak points of semidiscrete schemes. Just to mention a few, these include a poor resolution of contact discontinuities, and the development of spurious oscillations. These points can be improved, but the price to pay usually is a sharp increase in the computational cost. For this reason, it is interesting to explore adaptive strategies, where the scheme can be locally modified where needed, to increase its nonoscillatory properties or its resolution.

A more difficult task arises when dealing with applications. I've been discussing with a group interested in modelling vasculogenesis with chemiotactic models. In this case, a reliable numerical scheme can produce interesting results, but it is clear that the main problem is a lack of modelling. The same argument, I think, holds for say shallow water equations used in oceanography or multiphase flows, such as sprays. How can we use numerical computations to modify a model and improve its ability to predict phenomena?

A.20 Simeoni, Chiara

Hyperbolic conservation laws with source terms and constraints figure in many applications, especially as mathematical models for geophysical flows, and an incontestable importance is attached to the question of their numerical approximation from both a theoretical and practical viewpoint.

This brief contribution intends to reaffirm the interest in the main research objectives of the workshop in that field, by suggesting some relevant issues to be raised further and introducing specific problems which indicate the possibility of extending the techniques developed for the numerical modelling of hyperbolic conservation laws with source terms.

Numerical simulation of experimental data. Despite its simple configuration, the shallow water flow in channels with nontrivial topography is characterized by a wide variety of regimes, exhibiting some peculiar behaviours of the free-surface (wave trains, hydraulic jumps, turbulent profiles, ...), which have not yet been fully examined.

Due to the inherent limitations of the theoretical models, their predictions have to be interpreted in terms of experimental verifications, that leads to introduce more complex source terms for an accurate description of the empirical context.

The interaction of the source terms corresponding to the bottom topography and friction in the Saint-Venant equations for shallow water, for instance, is determinant of the appearance of steady states.

In numerical simulations of experimental data, it is rather difficult to reproduce correctly the steady states and to preserve this kind of solutions for a large number of time-steps, especially while dealing with transcritical flow regimes.

The focus on numerical schemes for shallow water equations with friction terms is motivated by the interest in recovering the results of experimental studies on the free-surface flows over complex topography [KS1] and some recent applications to the models of avalanches, in particular to describe the stopping mechanism of a granular mass in presence of Coulombtype friction terms [MVB].

A few specific methods to approximate the friction terms in the Saint-Venant equations have been developed, which present the common feature to be semi-implicit, as suggested by the specific nature of the friction term whose effects on the flow are observed all during the phenomena.

For the experimental framework, the question of the boundary conditions has also to be rigorously addressed, that is crucial for the computational accuracy with unstructured mesh in presence of source terms.

Those directions would be exploited to make further achievements in that field.

Incompressible Navier-Stokes equations. We are interested in the numerical modelling of the incompressible Navier-Stokes equations, in two space dimensions.

In the context of finite element methods, for instance, this problem leads to specific difficulties related to the treatment of the incompressibility condition, as the divergence-free constraint holds only weakly in the finite element spaces.

Moreover, in the limit of small viscosity, when the transport terms are dominant and the equations converge (at least formally) to the incompressible Euler equations, the error estimates become meaningless due to the general loss of stability of the numerical schemes.

The main idea of this contribution is to consider numerical schemes for the incompressible Navier-Stokes equations, based on finite volume or finite difference methods, with the

incompressibility condition (which turns out to be an algebraic constraint) treated as the steady state equations in the context of well-balanced schemes for conservation laws with source terms.

That approach is expected to provide stability properties, uniformly with respect to the diffusion parameters of the system, to prove error estimates and deduce the convergence of the numerical schemes to the (smooth) solutions of the incompressible Navier-Stokes equations.

That issue is particular important in the numerical modelling of the incompressible Navier-Stokes equations, because dealing with the divergence-free condition rigorously is still an open question [RR].

Some theoretical questions. The question of formulating appropriate consistency conditions for the Upwind Interface Source method [KPS] to prove error estimates in the general case of a non-uniform spatial mesh is particularly interesting, motivated by two-dimensional problems set on unstructured grids.

Some results in that direction have already been obtained in collaboration with Th. Katsaounis, most in the spirit of [KS2].

Bibliography

[KPS] Th. Katsaounis, B. Perthame, C. Simeoni, Upwinding sources at interfaces in conservation laws, *Appl. Math. Lett.* **17** (2004), no. 3, 309-316

[KS1] Th. Katsaounis, C. Simeoni, Second order approximation of the viscous Saint-Venant system and comparison with experiments, *Hyperbolic problems : theory, numerics, applications*, 633-644, Springer, Berlin, 2003

[KS2] Th. Katsaounis, C. Simeoni, First and second order error estimates for the upwind source at interface method, *Math. Comp.* **74** (2005), no. 249, 103-122

[MVB] A. Mangeney-Castelnau, J.P. Vilotte, M.O. Bristeau, F. Bouchut, B. Perthame, C. Simeoni, S. Yernini, A new kinetic scheme for Saint-Venant equations applied to debris avalanches, *INRIA Report RR-4646* (2002) – http://www.inria.fr/rrrt/rr-4646.html

[RR] R. Rannacher, Finite element methods for the incompressible Navier-Stokes equations, Fundamental directions in mathematical fluid mechanics, 191-293, Advances in Mathematical Fluid Mechanics, Birkhäuser Verlag, Basel, 2000

A.21 Tadmor, Eitan

We study the questions of global regularity vs. finite time breakdown in Eulerian dynamics, $u_t + u \cdot \nabla_x u = \nabla_x F$, subject to different source terms $F(u, \nabla u, D^2 u, ...)$. To address these questions, we propose the notion Critical Threshold (CT), where a conditional finite time breakdown depends on whether the initial configuration crosses an intrinsic, $\mathcal{O}(1)$ critical threshold. Our approach is based on the spectral dynamics of the eigenvalues, $\lambda := \lambda(\nabla u)$. We shall outline three prototype cases.

We begin with the *n*-dimensional restricted Euler equations, obtaining [n/2]+1 spectral invariants which surprising characterizations of critical thresholds in 3D and, in particular, 4D restricted Euler dynamics. Next we introduce the corresponding n-dimensional Restricted Euler-Poisson (REP) system, identifying a remarkable two-dimensional CT configurations with global REP smooth solutions. Finally we show how rotation prevents finite-time breakdown. Our study reveals the dependence of the CT phenomenon on the initial spectral gap, $\lambda_2(0) - \lambda_1(0)$.

A.22 Xing, Yulong

Hyperbolic balance laws have steady state solutions in which the flux gradients are nonzero but exactly balanced by the source term. Such cases, along with their perturbations, are very difficult to capture numerically. We are interested in finding such well-balanced schemes which are high order accurate for general solutions.

A typical example is the still water solution of the shallow water equation with a non-flat bottom topology. The equation takes the form

$$\begin{cases} h_t + (hu)_x = 0\\ (hu)_t + \left(hu^2 + \frac{1}{2}gh^2\right)_x = -ghb_x, \end{cases}$$
 (7)

with the still water solution:

$$h + b = constant$$
 and $hu = 0$. (8)

Recently, we have developed a well balanced high order finite difference WENO scheme [XS], and then generalized the result into high order finite volume schemes and discontinuous Galerkin methods [XS3]. In [XS2], we extend this idea to a general class of balance laws with separable source terms, allowing the design of well balanced high order scheme for all balance laws falling into this category. This class includes some steady state solutions of the elastic wave equation, the hyperbolic model for a chemosensitive movement, the nozzle flow and a two phase flow model.

We are also interested in preserving more general steady state solution exactly. For example, the shallow water equation has a more general steady state solution, which takes the form:

$$\frac{1}{2}u^2 + g(h+b) = constant \quad \text{and} \quad hu = constant.$$
 (9)

This is a pretty difficult problem and we are still working on it.

Bibliography

[XS] Y. Xing and C.-W. Shu, *High order finite difference WENO schemes with the exact conservation property for the shallow water equations*, Journal of Computational Physics, to appear.

[XS2] Y. Xing and C.-W. Shu, High order well-balanced finite difference WENO schemes for a class of hyperbolic systems with source terms, submitted to Journal of Scientific Computing. [XS3] Y. Xing and C.-W. Shu, High Order Well-balanced Finite Volume WENO Schemes and Discontinuous Galerkin Methods for a Class of Hyperbolic Systems with Source Terms, preprint.

A.23 Younis, Rami

See contribution of Margot Gerritsen.

A.24 Zeitlin, Vladimir

A fundamental problem in Geophysical Fluid Dynamics (GFD) is that of dynamical separation (non-interaction), or non-separation of fast and slow components of motion. The fast component is provided by waves and the slow one by vortices or jets. It is known that many utmostly important meteorological and climatic phenomena depend crucially on such (non-)separation. There are theoretical reasons for separation at small nonlinearities

in rotating stratified fluids, based on the asymptotic expansions (e.g. Reznik, Zeitlin and Ben Jelloul, 2001; Zeitlin, Reznik and Ben Jelloul, 2003). The question what happens at moderate/large nonlinearities is largely unanswered and should be adressed numerically. However, the fact of the presence of very different time- and space-scales in the problem renders numerical simulations difficult as they have to resolve well the small-scale fast waves and maintain balanced slow vortex motions quasi-stationary. In addition, wave-breaking should be properly resolved as it plays a crucial role in the wave-vortex interactions (e.g. Le Sommer, Reznik and Zeitlin, 2004). Wave-breakings of different nature may occur in GFD (Bouchut, Le Sommer and Zeitlin, 2005).

The simplest possible GFD model is rotating shallow water (RSW) equations. The Coriolis force enters the equations written as a system of conservation laws in a form of specific source which needs balancing. Recent progress in this model allows to obtain well-balanced schemes (Bouchut, 2004). The next in the hierarchy of the GFD models are models with superposition of several constant-density RSW layers, where the progress is much more difficult to make. The problem of well-balanced wave-breaking resolving numerical scheme is yet harder for full continuously stratified, so called "primitive", equations (PE) of the GFD. It should be noted that multi- or one-layer RSW models may be obtained by vertical averaging from the PE model.

References:

- F. Bouchut, "Nonlinear stability of finite volume methods for hyperbolic conservation laws and well-balanced schemes for sources", Birkhauser (2004).
- F. Bouchut, J. Le Sommer, V. Zeitlin, "Breaking of balanced and unbalanced equatorial waves", Chaos, to appear in 2005.
- J. Le Sommer, G.M. Reznik, V. Zeitlin, "Nonlinear geostrophic adjustment of long-wave disturbances in the shallow water model on the equatorial beta-plane" J. Fluid Mech., v. 515, 135 170 (2004).
- G.M. Reznik, V. Zeitlin, M. Ben Jelloul, "Nonlinear theory of the geostrophic adjustment. Part I. Rotating shallow water" -J. Fluid. Mech., v. 445, 93 120 (2001)
- V. Zeitlin, G.M. Reznik, M. Ben Jelloul, "Nonlinear theory of the geostrophic adjustment. Part II. Two-layer and continuously stratified models" J. Fluid. Mech., v. 491, 207 228 (2003)