Structure-Preserving Discretizations for Nonlinear Systems of Hyperbolic, Involution-Constrained Partial Differential Equations on Manifolds

Oberwolfach Workshop April 11 - 15, 2022

organized by:

Manuel Castro (Malaga)
Bruno Deprés (Paris)
Michael Dumbser (Trento)
Christian Klingenberg (Würzburg)

schedule with links to videos of the lectures

	Mo	Tue	Wed	Thur	Fr
9:00	9:00 opening 9:05 Brenier	Sonnendrücker	Barsukow	Dumbser	Dubois
9:45	9:50 Castro (online)	Despres	Barbara Re	Peshkov	Romensky (online)
10:30	10:35 *break*	*break*	*break*	*break*	*break*
11:00	Helluy	Crouseilles	Munz	Gavrilyuk	Pavelka
11:45	*break*	*break*	*break*	*break*	*break*
12:30	**lunch**	**lunch**	**lunch**	**lunch**	**lunch**
		15:30 Klingenberg			
16:00	Guermond	16:15 Birke	Oberwolfach hike	Busto	
16:45	*break*	17:00 *break*		*break*	
17:15	Puppo	17:30 Gaburro		Shashkov (online)	
18:00	*break*	18:15 *break*		*break*	
18:30	**dinner**	**dinner**	**dinner**	**dinner**	**dinner**

Participants:

Barsukow, Wasilij, *Garching bei München (DE)*
Birke, Claudius, *Würzburg (DE)*
Brenier, Yann, *Paris (FR)*
Busto, Saray, *Madrid (ES)*
Castro Diaz, Manuel J., *Malaga (ES)* (online)
Chandrashekar, Praveen, *Bangalore, Bengaluru (IN)* (online)
Crouseilles, Nicolas, *Rennes (FR)*
Després, Bruno, *Paris (FR)*
Dubois, François, *Orsay (FR)*
Dumbser, Michael, *Trento (IT)*
Gaburro, Elena, *Talence (FR)*
Gassner, Gregor, *Köln (DE)* (online)
Gavrilyuk, Sergey L., *Marseille (FR)*
Guermond, Jean-Luc, *College Station (US)*
Helluy, Philippe, *Strasbourg (FR)*
Klingenberg, Christian, *Würzburg (DE)*
LeFloch, Philippe G., *Paris (FR)* (online)
Munz, Claus-Dieter, *Stuttgart (DE)*
Pavelka, Michal, *Praha (CZ)*
Peshkov, Ilya, *Trento (IT)*
Puppo, Gabriella, *Roma (IT)*
Re, Barbara, *Milano (IT)*
Romensky, Evgeniy, *Novosibirsk (RU)* (online)
Shashkov, Mikhail, *Los Alamos (US)* (online)
Sonnendrücker, Eric, *Garching bei München (DE)*

Schedule

MONDAY, APRIL 11

9:05 am **Brenner, Yann** (Paris, France)

Title: Structural similarities between the isothermal Euler equations and the Einstein equations in vacuum with a cosmological constant

Abstract: The Einstein equations in vacuum with a cosmological constant can be interpreted as a matrix-valued generalization of the isothermal Euler equations, for which the speed of sound is constant. The similarity between the two equations is obtained through the least action principle. We may even include the free Schroedinger equation in the same framework, through the Madelung transform.

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9:50 am **Castro, Manuel** (Malaga, Spain):

Title: High oder Implicit and semi-implicit well-balanced finite volume schemes for balance laws

Abstract: The goal of this work is to design implicit and semi-implicit high-order well-balanced numerical methods for systems of balance laws with stiff numerical flux and source term. Here we use the general strategy introduced by Castro-Pares (2020) to construct high-order well-balanced reconstruction operators that are combined with standard RK-IMEX or RK-Implicit to integrate in time the balance laws. We will show that strategy that we propose is able to maintain the properties of the RK-IMEX and RK-implicit method design for the homogenous system and the well-balanced property of the reconstruction operator, ensuring the well-balanced character of the resulting methods. This general strategy will be applied to several systems of balance laws, such as the Burgers equation with source term or the 1D shallow water system.

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11:00 am **Helluy, Philippe** (Strasbourg, France):

Title: Quasi-explicit, unconditionally stable, time solvers for conservation laws

Abstract: We describe a parallel and quasi-explicit Discontinuous Galerkin (DG) kinetic scheme for solving hyperbolic systems of conservation laws. The solver is unconditionally stable (i.e., the CFL number can be arbitrary), has the complexity of an explicit scheme. The time integration can be fully time reversible. It can be applied to any hyperbolic system of balance laws. In this work, we assess the performance of the scheme in the particular cases of the Maxwell's equations. We measure the benefit of the unconditional stability by performing experiments with very large CFL numbers. In addition, the parallel possibilities of the method are investigated.

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4:00 pm **Guermond, Jean-Luc** (College Station, USA):

Title: Invariant-domain preserving high-order implicit-explicit time stepping: Beyond the SSP paradigm

Abstract: We consider high-order discretizations of a Cauchy problem where the evolution operator comprises a hyperbolic part and a parabolic part with diffusion and stiff relaxation terms. We propose a technique that makes every implicit-explicit (IMEX) time stepping scheme invariant domain preserving and mass conservative. Following the ideas introduced in Part I on explicit Runge--Kutta schemes, the IMEX scheme is written in incremental form and, in each stage of the scheme, we first compute low-order hyperbolic and parabolic updates, followed by their high-order counterparts. The proposed technique, which is agnostic to the space discretization, allows to optimize the time step restrictions induced by the hyperbolic sub-step. To illustrate the proposed methodology, we derive three novel IMEX schemes with optimal efficiency and for which the implicit scheme is singly-diagonal and L-stable: a third-order, four-stage scheme; and two fourth-order schemes, one with five stages and one with six stages. The novel IMEX schemes are evaluated numerically on a stiff ODE system, and their explicit component is also tested on hyperbolic problems. In the third part of this work, we show how to apply these schemes to nonlinear convection-diffusion problems with stiff reaction and to compressible viscous flows possibly including grey radiation.

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5:15 pm **Puppo, Gabriella** (Rome, Italy):

Title: Going implicit: large time steps for hyperbolic systems

Abstract: In recent years we have witnessed a large body of research concentrated on Low Mach problems. The idea is that in many applications propagation phenomena induced by hyperbolic systems are characterized by very different speeds, and the phenomenon of interest is carried by low speed waves. In gas dynamics this typically occurs in almost incompressible flow, where the acoustic waves are much faster than material waves. In these cases, the classical CFL condition of explicit schemes forces small time steps, even though one is really interested in the advection of material waves.
In this talk I will skim through the issues behind the construction of Low Mach schemes, and a few solutions on which I have worked.
In the second part of the talk, I will discuss some problems which still need to be addressed. In particular, I will try to outline the difficulties behind the construction of fully implicit schemes for hyperbolic systems. In fact, most if not all Low Mach schemes are problem-specific. I will end with the description of a scheme we are proposing which is a sort of black box high order implicit scheme for hyperbolic problems.

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TUESDAY, APRIL 12

9:00 am **Sonnendrücker, Eric** (Garching, Germany)

Titel: Hamiltonian plasma physics models and their discretization

Abstract: Many models in plasma physics can be derived from a non canonical hamiltonian formulation expressed using a Poisson bracket and a conserved Hamiltonian. For long time simulations, conservation of invariants coming from the hamiltonian formulation are essential. This can be achieved in particular by looking for a discrete Poisson bracket and Hamiltonian and then using splitting of either the bracket or the hamiltonian. As examples we will consider the Vlasov-Maxwell equations as well as hybrid fluid-kinetic models. We shall also show how dissipative effects can be added using a symmetric positive non definite bracket and a dissipated entropy.

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9.45 am **Després, Bruno** (Paris, France):

Title: Reduction of a magnetized Vlasov equation as a Friedrichs system

Abstract: The calculation of numerical solutions to kinetic equations in plasmas (often modeled as Vlasov equations) is arguably a formidable task. In magnetized plasmas, there is the possibility to use gyrokinetic equations so as to reduce the dimension of the problem and to reduce the computational burden. It appears that Vlasov equations can be seen as infinite dimensional Friedrichs equations by using a convenient moment approach.
I will report on recent advances obtained within the ANR projet MUFFIN. The main difficulty is to construct moments which are adapted to direction of the (strong) magnetic field. One obtains finite dimensional Friedrichs systems. It is possible to pass to the limit for strong magnetic field. One obtains reduced models which can be compared with gyrokinetic models. It appears that the Friedrichs models are richer since they incorporate the curvature of the magnetic field. Numerical methods are easily developed with standard tools and some results will be shown.
Thanks to Muffin participants, in particular R. Dai (postdoc), F. Charles (SU) and S. Hirstoaga (Inria).

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11:00 am **Crouseilles, Nicolas** (Rennes, France):

Titel: High Order Numerical Methods for a Hybrid Kinetic/Fluid Plasma Model

Abstract: In this talk, we will focus on the numerical approximation of a hybrid fluid-kinetic plasma model for electrons, in which energetic electrons are described by a Vlasov kinetic model whereas a fluid model is used for the cold population of electrons.
First, we study the validity of this hybrid modeling in a two-dimensional context (one dimension in space and one dimension in velocity) against the full (stiff) Vlasov kinetic model and second, a four-dimensional configuration is considered (one dimension in space and three dimensions in velocity).
To do so, we consider two numerical Eulerian methods. The first one is based on the Hamiltonian structure of the hybrid system and the second approach, which is based on exponential integrators, enables to derive high order integrator and remove the CFL condition induced by the linear part.
The efficiency of these methods, which are combined with an adaptive time stepping strategy, are discussed in the different configurations and in the linear and nonlinear regimes.
This is a joint work with A. Crestetto (University Nantes) and J. Massot (Ecole Polytechnique).

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3:30 pm **Klingenberg, Christian** (Würzburg, Germany)

Title: Structure preserving numerical methods in a multi-scale context

Abstract: This lecture will focus on the compressible Euler equations with gravity, seen together with its incompressible limit. Numerical schemes that manage to follow these limits are studied together with their ability to maintain stationary solutions. It is important to pay attention to their interplay.

This is joint work with among others Wasilij Barsukow, Claudius Birke and Fritz Röpke.

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4:15 pm **Birke, Claudius** (Würzburg, Germany)

Title: A well-balanced and asymptotic preserving relaxation scheme for the Euler equations with gravity

Abstract: We present a numerical approximation of the solutions of the Euler equations with a gravitational source term. Based on a Suliciu-type relaxation model with two relaxation speeds, we construct an approximate Riemann solver, which is used in a first order Godunov-type finite volume scheme. A Mach number dependent scaling of the relaxation speeds prevents excessive dissipation in the low Mach regime and leads to a provably asymptotic-preserving method. In order to preserve stationary solutions, we include the gravitational potential in the approximate Riemann solver. As a result, the solver maintains any hydrostatic equilibrium to second order, special families of equilibria and a-priori known hydrostatic solutions even up to machine precision. In addition, our solver has other typical properties of relaxation solvers: it is positivity-preserving for both density and internal energy, and furthermore satisfies a discrete form of the entropy inequality. Using this entropy inequality, it can be proven that the scheme guarantees not to give rise to numerical checkerboard modes in the incompressible limit. The scheme can be extended to second order without loosing its properties. We illustrate the schemes properties in numerical tests.

This is joint work with Christophe Chalons (Versailles) and Christian Klingenberg (Würzburg).

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5:30 pm **Gaburro, Elena,** (Talence, France)

Title: Well balanced finite volume scheme for covariant hyperbolic systems

Abstract: The aim of this talk is to present a novel second order accurate well balanced (WB) finite volume (FV) scheme for the solution of covariant hyperbolic systems. In particular, we will focus on the general relativistic magnetohydrodynamics (GRMHD) equations and the first order CCZ4 formulation (FO-CCZ4) of the Einstein field equations of general relativity, as well as the fully coupled FO-CCZ4 + GRMHD system. These systems of first order hyperbolic PDEs allow to study the dynamics of the matter and the dynamics of the space-time according to the theory of general relativity.

The new well balanced finite volume scheme exploits the knowledge of an equilibrium solution of interest when integrating the conservative fluxes, the nonconservative products and the algebraic source terms, and also when performing the piecewise linear data reconstruction. This results in a rather simple modification of the underlying second order FV scheme, which, however, being able to cancel numerical errors committed with respect to the equilibrium component of the numerical solution, substantially improves the accuracy and long-time stability of the numerical scheme when simulating small perturbations of stationary equilibria. In particular, the need for well balanced techniques appears to be more and more crucial as the applications increase their complexity.

We close the presentation with a series of numerical tests of increasing difficulty, where we study the evolution of small perturbations of accretion problems and of stable TOV neutron stars, and with an outlook on our future research directions, which includes other covariant hyperbolic systems that can be considered using this formalism.

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WEDNESDAY, APRIL 13

9:00 am **Barsukow, Wasilij** (Garching, Germany)

Title: Active Flux, a numerical method with global continuity

Abstract: Active Flux is a novel numerical method for hyperbolic conservation laws, going back to van Leer, 1977 and Eymann & Roe, 2013. Its classical degrees of freedom are cell averages and point values at cell interfaces. Most importantly, these latter are shared between adjacent cells, leading to a globally continuous reconstruction -- the distinctive feature of Active Flux. The update of the point values includes upwinding, but without solving a Riemann Problem. The update of the cell average requires a flux quadrature at the cell interface, which can be immediately performed using the point values. This approach, different from Finite Volume, DG and continuous Finite Element methods, is stable, allows to resolve shocks and has a number of further favorable properties. For example, it has been shown to be stationarity and vorticity preserving for the acoustic equations in multiple spatial dimensions, where an exact evolution operator includes all the multi-dimensional information in the point value update. It also allows to use different formulations of the same conservative PDE for the different degrees of freedom.

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9:45 am **Re, Barbara** (Milano, Italy)

Title: A pressure-based model for two-phase flows with pressure and velocity disequilibrium under generic equations of state

Abstract: Transient compressible two-phase flows exhibit a complex multi-scalse neature. Diffuse interface methods represent a popular strategy to model such flow fields, which considers a small, artificial mixing of the fluids at the otherwise resolved interface. These methods are based on augmented systems of governing equations, which include suitable transport terms to account for the interaction between phases.

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11:00 am **Munz, Claus-Dieter** (Stuttgart, Germany)

Title: Godunov-type Numerical Fluxes for Diffusion

Abstract: For finite volume or discontinuous Galerkin schemes, the use of the exact or approximate Riemann solution to construct the numerical fluxes is a standard approach that started with the work of Godunov. Gassner et al. initiated the use of the Riemann problem solution to construct diffusive fluxes later in [1]. However, the more common approach is still to reconstruct the necessary gradients for the diffusive fluxes by assuming continuity across the grid cell interface. This is motivated by the regularizing property of the parabolic terms. I revisit the Godunov-type approach for the sharp interface approximation of two-phase flow. Here, the phase interface is approximated as a discontinuity within the macroscopic description. This structure is preserved in the construction of the heat flux or the viscous fluxes across the interface. In the talk, I review the old work of the construction of numerical fluxes based on the generalized diffusive Riemann problem. Then I discuss its use at phase or material interfaces and show some results for validation and applications.
[1] G. Gassner, F. Lörcher, C.-D. Munz, "A contribution to the construction of diffusion fluxes for finite volume and discontinuous Galerkin schemes", Journal of Computational Physics 224 (2007) 1049-1063.

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THURSDAY, APRIL 14

9.00 am **Dumbser, Michael** (Trento, Italy)

Title: Dealing with curl involutions in Newtonian continuum mechanics and general relativity

Abstract:

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9:45 am **Peshkov, Ilya** (Trento, Italy)

Title: The role of curl-type involutions in continuum physics

Abstract: In the nonlinear elasticity theory, the curl of the strain field vanishes and is known as the so-called compatibility condition, which, if holds initially, should stay so for all later times. This is a typical example of a curl-type involution constraint. In this talk, we generalize this idea and show that this spatial involution constraint is in fact a projection of a space-time identity. We then briefly discuss that this observation is not unique to the elasticity theory and can be met for example in the so-called Yang-Mills gauge theory. We also discuss that this observation might be used for constructing involution-preserving numerical methods and for modeling of some phenomena such as turbulence, or wave propagation in complex solids (i.e. solids with (with internal microstructure).

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11:00 am **Gavrilyuk, Sergey L.** (Marseille, France):

Title: Generalized Rankine -- Hugoniot relations for multi-D shocks in dispersive media

Abstract: We study a class of Euler-Lagrange equations describing waves in dispersive media. We show that, contrary to popular belief, disppersive regularization does not exclude the development of localized shock-like transition fronts. The Rankine-Hugoniot relations across such fronts are derived. They are consequences of the corresponding conservation laws complemented by additional relations coming from the variational formulation of the governing equations. Applications to compressible fluids with internal capillarity and to bubbly liquids are discussed. Such generalized Rankine-Hugoniot relations should probably be implemented in the numerical schemes solving these Euler-Lagrange equations.

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4:00 pm **Busto, Saray** (Madrid, Spain):

Title: Thermodynamically compatible finite volume schemes for continuum mechanics

Abstract: In this talk, we will present a novel discretization of the Godunov-Peshkov-Romenski model (GPR model) for continuum mechanics. This hyperbolic and thermodynamically compatible PDE system is able to describe from nonlinear elastoplastic solids at large deformations to viscous fluids at the aid of suitable relaxation source terms making it a powerful tool to model numerous physical phenomena. One of the main challenges on the development of numerical methods for this kind of systems consists on preserving the thermodynamically compatibility of the equations also at the discrete level. To this end, we will start constructing a discrete framework for the compressible Euler equations mimicking the

continuous formalism introduced by Godunov in 1961. The remaining terms in the more general GPR model, including non-conservative products, will be then carefully discretized to achieve discrete thermodynamic compatibility, with the exact conservation of total energy density as a direct consequence of all the other equations. Moreover, we will see that the HTC scheme proposed is provably marginally stable in the energy norm and satisfy a discrete entropy inequality by construction. We will finally analyze some numerical test assessing the behavior of the proposed methodology both in the solid and fluid limits.

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5:15 pm **Shashkov, Mikhail** (Los Alamos, USA):

Title: Modern numerical methods for high-speed, compressible, multi-physics, multi-material flows

Abstract: This is an overview lecture.

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FRIDAY, APRIL 15

9:00 am **Dubois, François** (Orsay, France)

Title: A result of convergence for a one-dimensional two-velocities lattice Boltzmann scheme

Abstract: In this lecture, we introduce the underlying ideas of lattice Boltzmann schemes to colleagues that are not familiar with this. We present also briefly one of the first results, obtained with Filipa Caetano and Benjamin Graille, concerning the convergence of lattice Boltzmann schemes in a nonlinear context.

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9:45 am **Romensky, Evgeniy** (Novosibirsk, Russia)

Title: Hyperbolic thermodynamically compatible model for wave processes in a deformed porous medium saturated with multiphase mixture

Abstract: A new approach to modeling a saturated deformable porous medium considered as a multiphase mixture based on the theory of symmetric hyperbolic thermodynamically consistent systems is discussed.
A model is presented that takes into account finite deformations of a skeleton saturated with a mixture of compressible fluids and gases. The model makes it possible to take into account the viscosity of the saturating fluid and the inelastic deformations of the porous medium. The governing PDEs of the model satisfy the laws of nonequilibrium thermodynamics and form a symmetric hyperbolic system with stiff source terms and curl involutions. The structure of the equations, which include equations for the phase volume fractions, makes it possible to apply the diffuse interface method to simulate processes in a region with inclusions of pure elastic medium or pure fluid. In this case, the interphase boundary is modeled by a jump in volume fraction.

Linearized equations of the model are formulated for simulation the propagation of small amplitude waves in a saturated porous medium. A series of numerical calculations demonstrating the capabilities of the model is presented.

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11:00 am **Pavelka, Michal** (Prague, Czech Republic)

Title: Hamiltonian mechanics leads to hyperbolic partial differential equations

Abstract: The principle of stationary action can be reformulated as Hamiltonian mechanics, where evolution is generated by a Poisson bracket and energy. Here, we show that Hamiltonian continuum mechanics typically leads to first-order hyperbolic partial differential equations (for instance to fluid mechanics). Moreover, Hamiltonian mechanics reveals extra structures of the equations (for instance the Jacobi identity, or Riemannian geometry of the state space), that can be used in further generalizations or when constructing numerical solvers. In particular, the reversible part of the Symmetric Hyperbolic Thermodynamically Compatible equations (SHTC) is Hamiltonian, which helps to generalize the framework in case of binary mixtures or superfluid helium-4. It seems also that the Hamiltonian structure may lead to geometric structure-preserving Hamiltonian solvers for the equations, similar to the smoothed particle hydrodynamics (SPH) method.

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