

# Workshop Progetto GNCS 2019

## Numerical approximation of hyperbolic problems and applications

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### Abstracts

Giacomo Albi  
Università di Verona

*Multistep methods for hyperbolic relaxation system and optimal control problems*

We are interested in high-order multistep schemes for time discretization of hyperbolic systems with relaxation. More specifically, we consider hyperbolic balance laws in which the convection and the source term may have very different time and space scales. As a consequence the nature of the asymptotic limit changes completely, passing from a hyperbolic to a parabolic system. In this context we are concern with optimal control problems and their applications. First considering optimal control problems for ordinary differential equations and show loss of accuracy for Adams-Moulton and Adams-Bashford methods, whereas BDF methods preserve high-order accuracy. Subsequently we extend these results to semi-lagrangian discretizations of hyperbolic relaxation systems. Computational results illustrate theoretical findings.

Clarissa Astuto  
Università di Catania

*Multi-scale modeling of Sorption Kinetics*

The trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of different real problems in chemistry, physics and biology. Here we study the dynamics of diffusing particles in a domain with an oscillating bubble. Laboratory experiments provide evidence of a non monotone behavior in time of the concentration of particles by a detector located behind the bubble, under suitable experimental condition. A comprehensive explanation of the phenomenon is not yet fully available. The particles are attracted and trapped near the surface of the bubble. The basic mathematical model is a drift-diffusion model, where the particles diffuse and feel the potential of the bubble when they are near its surface. The numerical simulation of the system presents two multi-scale challenges. One is spatial: the range of the bubble potential is confined within a few microns at the bubble surface, while the bubble radius is of the order of a millimeter, so a fully resolved solution would be too expensive. The second challenge is on the time scale: the bubble oscillates with

a frequency of the order of 100 Hz, while the diffusion time scale is of the order of 103 seconds, this requiring at least 106 time steps to fully resolve the problem in time. A reduced model is derived to solve the multi-scale problem in space: the interaction with the bubble is modeled as a very thin layer, with a particle surface density proportional to the local density in the bulk, near the bubble. In the rest of the domain the particle density satisfies just a diffusion equation, with suitable boundary conditions on the bubble, deduced from conservation properties. The model is carefully tested on problems in 1D, 2D planar and 3D axis-symmetric geometry. The equation is discretized on a regular Cartesian mesh, using a ghost-point approach, and solved by Crank-Nicolson scheme. The implicit step is efficiently solved by a suitably adapted multi-grid method. The amplitude of the bubble oscillations is small compared to the bubble radius. We take advantage of this fact by replacing the time dependent position by imposing a suitable time dependent velocity at the bubble surface. Because of the low Reynolds number, the velocity distribution is computed by Stokes approximation. The multi-scale challenge in time is still under investigation.

Caterina Bassi  
Politecnico di Milano

*A new hyperbolic reformulation of the Serre-Green-Naghdi model for general bottom*

The phenomenon we are interested in is the propagation of sea waves near the coast: in this context the vertical length scale is much smaller than the horizontal one and the shallow water approximation can be successfully employed. We are however interested in dispersive water waves, which can not be captured by the classical hydrostatic shallow water equations. In this framework, we propose a new hyperbolic reformulation of the non-hydrostatic Serre-Green-Naghdi system without the mild bottom approximation. We present a derivation of this new system obtained by vertically averaging the compressible Euler equations, we show that the system is strictly hyperbolic and that it satisfies an energy conservation law, which reduces to the energy conservation law associated to the original SGN system when a suitable parameter (which represents an artificial sound speed) goes to infinity. Thanks to the hyperbolicity, the model has been implemented in an ADER-DG numerical scheme in a very straightforward way. Different testcases, both with flat bottom and with varying bottom, show that the proposed model correctly reproduces numerical and experimental results already present in the literature.

Tommaso Benacchio  
Politecnico di Milano

*A Semi-Implicit Compressible Model for Atmospheric Flows with Seamless Access to Soundproof and Hydrostatic Dynamics*

Atmospheric flows develop on a wide range of spatial and temporal scales with dynamics generally modelled with the compressible Euler equation. In this context, fast gravity waves and acoustics are deemed unimportant for weather prediction of synoptic-scale systems, yet stiffen the numerics through stability-driven time steps constraints. We present results with a second-order semi-implicit finite-volume method for the simulation of compressible fluid flow equations in the low Mach number regime. The model is written in conservation form and uses a combination of implicit midpoint and implicit trapezoidal time integration to achieve time steps unconstrained by the speed of both gravity waves and acoustic waves. In

addition, the scheme can be written in terms of full variables or perturbations with no accuracy variation, and with switches to the pseudo-incompressible and hydrostatic dynamical models valid in the small-scale and large-scale limits. Model performance is tested on thermal perturbations and inertia-gravity waves at increasingly large scales and with different model configurations. We show that the scheme can flexibly operate the same numerics on different equation sets with uniform accuracy and efficiency, and propose applications in the framework of balanced data assimilation.

Walter Boscheri  
Università di Ferrara

*A second order all Mach number IMEX finite volume solver for the three dimensional Euler equations*

This article deals with the development of a numerical method for the compressible Euler system valid for all Mach numbers: from extremely low to high regimes. In classical fluid dynamic problems, one faces both situations in which the flow is subsonic, and consequently acoustic waves are very fast compared to the velocity of the fluid, and situations in which the fluid moves at high speed and compressibility may generate shock waves. Standard explicit fluid solvers such as Godunov method fail in the description of both flows due to time step restrictions caused by the stiffness of the equations which leads to prohibitive computational costs. In this work, we develop a new method for the full Euler system of gas dynamics based on partitioning the equations into a fast and a low scale. Such a method employs a time step which is independent of the speed of the pressure waves and works uniformly for all Mach numbers. Cell centered discretization on Cartesian meshes is proposed. Numerical results up to the three dimensional case show the accuracy, the robustness and the effectiveness of the proposed approach.

Saray Busto Ulloa  
Università di Trento

*A hybrid FV/FE method for weakly compressible flows*

The aim of this talk is to introduce a novel semi-implicit hybrid finite volume-finite element method for the simulation of low Mach number flows on unstructured staggered grids. Classical compressible Navier-Stokes equations are rewritten in a velocity-pressure formulation and discretized in time resulting on the decoupling of pressure and momentum computations. Furthermore, space discretization is performed using staggered grids of the face-type built on a primal mesh of triangles/tetrahedra. Within the transport-diffusion stage of the projection algorithm, the advection-diffusion dominated equations are solved explicitly using a finite volume method. Second order of accuracy in space and time is attained applying ADER methodology. Moreover, a path-conservative scheme is employed to deal with non-conservative products. The projection stage is devoted to the resolution of the pressure system using a finite element algorithm. Next, momentum variables are corrected using the pressure at the new time instant and the temperature field is recovered. Classical benchmarks are employed to assess the proposed methodology including the resolution of

Taylor-Green vortex, heat conduction and explosion problems.

Joint work with A. Bermúdez, M. Dumbser, L. Saavedra, J.L. Ferrín and M.E. Vázquez-Cendón.

Simone Cacace

Università di Roma Tre

*A Mean Field Game model for Cluster Analysis*

Cluster analysis is a typical task in unsupervised Machine Learning: given a data set of points in some metric space, find a partition into subgroups (clusters) such that the elements in each group are, in a suitable sense, more similar to each other than to those in other groups. Several algorithms, based on finite dimensional optimization techniques, have been proposed to perform clustering, and they are usually divided in two classes, hard and soft methods. In hard-clustering, as for the K-means algorithm, each data point can belong to a single cluster, whereas in soft-clustering, as for the Expectation-Maximization (EM) algorithm, each data point has a certain probability to belong to each cluster. In this talk, I will present an extension of the cluster analysis to the infinite dimensional setting, in which a "big data" set can be represented by a continuous density function. I will show that the problem can be interpreted as a stationary multi-population Mean Field Game (MFG), and I will discuss some details on the numerical approximation and solution of the corresponding MFG system. Finally, I will present some numerical results for classical clustering examples. This is a joint work with Laura Aquilanti, Fabio Camilli and Raul De Maio.

Elisa Calzola

Sapienza Università di Roma

*A second order semi-Lagrangian discretization of the advection-diffusion-reaction equation.*

Advection-diffusion-reaction equations have a multitude of applications, such as in climate, water and air quality models, or in short and medium range weather forecasting. Due to the potentially very large number of equations of this kind that have to be solved in order to describe such physical processes, every efficiency gain in the numerical discretization used for this very classical problem is of great practical importance. We propose a fully semi-Lagrangian method for the numerical solution of advection-diffusion-reaction equations that employs a second order semi-Lagrangian scheme. Standard interpolation procedures are used for reconstructing the solution in the foot of the characteristics, using both structured and unstructured meshes for the space discretization. We also propose a numerical treatment of Dirichlet boundary conditions. The method allows for large time steps, while avoiding the solution of large linear systems, since it follows an explicit approach. The work is completed by numerical experiments that demonstrate the effectiveness of the proposed approach.

Seung Yeon Cho  
Università di Catania

*A conservative reconstruction and its applications*

In this talk, I will introduce a conservative reconstruction which enables to design conservative semi-Lagrangian (SL) finite difference methods for transport-type equations. Applicable examples such as non-splitting SL schemes for BGK model and splitting SL methods for Vlasov-Poisson system will be dealt with in the presentation. The performance of conservative reconstructions applied to the SL methods will be confirmed by several numerical tests. This is a joint work with Prof. Giovanni Russo (UNICT), Prof. Sebastiano Boscarino (UNICT), and Prof. Seok-Bae Yun (SKKU).

Michael Dumbser  
Università di Trento

*A structure-preserving staggered semi-implicit scheme for continuum mechanics*

In this talk, we present a new class of structure-preserving semi-implicit schemes for the unified first order hyperbolic model of Newtonian continuum mechanics proposed by Godunov, Peshkov and Romenski (GPR). The GPR model is a geometric approach to continuum mechanics, which is able to describe the behavior of moving elasto-plastic solids as well as viscous and inviscid fluids within one and the same governing PDE system. This is achieved via appropriate relaxation source terms in the evolution equations for the distortion field and the thermal impulse. In previous work it has already been shown that the GPR model reduces to the compressible Navier-Stokes equations in the stiff relaxation limit when the relaxation times tend to zero. The governing PDE system belongs to the class of symmetric hyperbolic and thermodynamically compatible systems (SHTC), which have been studied for the first time by Godunov in 1961 and later in a series of papers by Godunov & Romenski. An important feature of the proposed model is that the propagation speeds of all physical processes, including dissipative processes, are finite.

In the absence of source terms, the homogeneous part of the GPR model is endowed with some natural involutions, namely the distortion field  $A$  and the thermal impulse  $J$  need to remain curl-free. In this talk we present a new structure-preserving scheme that is able to preserve the curl-free property of both fields exactly also on the discrete level. This is achieved via the definition of appropriate and compatible discrete gradient and curl operators on a judiciously chosen staggered grid. Furthermore, the pressure terms are discretized implicitly in order to capture the low Mach number limit of the equations properly, while all other terms are discretized explicitly. In this manner, the resulting pressure system is symmetric and positive definite and can be solved with efficient iterative solvers like the conjugate gradient method. Last but not least, the new staggered semi-implicit scheme is also able to reproduce the stiff relaxation limit of the governing PDE system properly, recovering an appropriate discretization of the compressible Navier-Stokes equations. To the best of our knowledge, this is the first pressure-based semi-implicit scheme for nonlinear continuum mechanics that is able to preserve all involutions and asymptotic limits of the original governing PDE system also on the discrete level. Computational results for several test cases are presented in order to illustrate the performance of the new scheme. Joint work with W. Boscheri, M. Ioriatti, I. Peshkov, E. Romenski.

Elisa Iacomini  
Sapienza Università di Roma

*Stop and Go waves: from a microscopic to a macroscopic description*

In this talk, different approaches in modelling Stop & Go waves (S&G) will be presented. This phenomenon is typical of congested traffic and have negative effects on safety, fuel consumption and air pollution. Nowadays it is very hard to find simulations which reproduce well recognizable S&G waves. Since modelling properly this phenomenon is crucial for developing techniques aimed at reducing it, we present three different approaches able to reproduce S&G waves, based on different scales of observation. We will develop a new microscopic second order model specially conceived to reproduce S&G waves, calibrated and validated by real data. Then we will couple the microscopic with a macroscopic model in order to recover S&G waves at a macroscopic level too. Lastly, we will introduce a time-delay in a first order macroscopic model to have a fully macroscopic description.

Emanuele Macca  
Università di Catania

*An order-adaptive compact approximation Taylor method for systems of conservation laws*

We present an order-adaptive finite difference numerical method for systems of conservation laws. The method, called Adaptive Compact Approximation Taylor method (ACAT), uses centered  $(2p + 1)$ -point stencils, where  $p$  may take values in  $\{1, 2, \dots, p_{max}\}$  according to a family of smoothness indicators in the stencils. The method is a combination between a robust first order scheme and  $2p$ -order generalized Lax-Wendroff methods, so that it is first order near shocks and of order  $2p$  in smooth regions, where  $(2p + 1)$  is the size of the biggest stencil in which large gradients are not detected. A new class of smooth indicators and the stability analysis will be presented. For nonlinear problems, the original LW procedure requires the conversion of the time derivatives to spatial derivatives through the so-called Cauchy-Kovalevskaya process, what may increase dramatically the computational cost. To avoid this, we adapt the Compact Approximate Taylor Method (CAT), by including an adaptive formulation in the numerical differentiation formulas plus a new class of smoothness indicators. In comparison with the Approximate Taylor methods presented, WENO flux reconstructions are not needed and values of the  $CFL$  parameter close to 1 can be used, which reduces significantly the computational cost. The general structure of the method and a number of numerical tests will be shown, in which the results are compared with those provided by standard WENO methods and the Approximate Taylor methods.

Giulio Paolucci  
Sapienza Università di Roma

*Multidimensional smoothness indicators for first order Hamilton-Jacobi equations*

The lack of smoothness is a common feature of weak solutions of nonlinear hyperbolic equations and it is a crucial issue in their approximation. This has motivated several efforts in order to devise appropriate indicators which aim is to detect the singularity regions of the domain and let the numerical scheme adapt according to the local regularity of the solution, reducing the formation of spurious oscillations when high-order discretizations are

employed. ENO and WENO approaches are typical examples. In this talk we focus on Lipschitz continuous functions and the goal is to detect the cells containing a jump in the gradient. We generalize the WENO approach to structured two-dimensional grids, overcoming the limitations of indicators based on dimensional splitting. Our indicators allow for the construction of multidimensional adaptive filtered schemes that we use to get an accurate approximation of viscosity solutions of first-order Hamilton-Jacobi equations. Filtered schemes are based on a simple coupling between a monotone scheme and a (possibly) unstable high-order scheme and are able to exploit the good features of both discretizations, achieving convergence and high-order consistency. Several numerical examples are presented that testify the reliability of the indicators and the related numerical scheme. This is a joint work with M.Falcone and S.Tozza.

Lorenzo Pareschi  
Università di Ferrara

*Consensus based optimization methods*

Over the last decades, large systems of interacting particles (or agents) have been widely used to investigate self organization and collective behavior. Similar particle models are used in metaheuristics (Particle swarm optimization, simulated annealing, etc.), which provides empirically robust solutions to tackle hard optimization problems with fast algorithms. Despite the tremendous empirical success of these techniques, most metaheuristic methods still lack proper mathematical foundations, like proof of robust convergence to global minimizers. Recently, methods inspired by consensus based models including a deterministic alignment and a stochastic Brownian noise have been successfully introduced in order to establish a consensus among particles on the location of the global minimizers within a certain domain. The evolution of the system can be interpreted as a classical first order stochastic differential equation, whose large particle limit is approximated by a deterministic partial differential equation of mean-field type. The large time behavior of such a deterministic PDE can be analyzed by classical techniques of large deviation bounds and the global convergence of the mean-field model to global minimizers can be mathematically proven in a rigorous way for a large class of optimization problems. Several applications to machine learning problems are also presented. (Joint research with M. Fornasier, H. Huang, P. Sunnen)

Gabriella Puppo  
Sapienza Università di Roma

*Numerical integration of Low Mach problems via relaxation*

Low Mach problems arise in gas dynamics when the local speed is much smaller than the acoustic waves. Similar problems arise also in elasticity, when the elastic waves are much slower than the acoustic waves. In these regimes, a full resolution of all the waves requires very small time steps, while usually one is interested only in the material waves. Standard implicit techniques do not require stability restrictions on the time steps, but they may require the solution of large non linear algebraic systems, and often they inject a spurious viscosity which does not permit to recover the correct asymptotic limits. In this work, we use relaxation to separate the different scales, and integrate implicitly only in the fast scales. We also prove that we recover the correct asymptotic limits, if the initial data are

close to the vanishing Mach limit, which yields the incompressible equations. We describe a first approach, based on the relaxation approach of Xi-Jin, and a different solution, obtained through a Suliciu like relaxation, in which only the pressure terms undergo relaxation.

Giovanni Russo  
Università di Catania

*Multi-scale numerical modeling of sorption kinetics*

The trapping of diffusing particles by either a single or a distribution of moving traps is an interesting topic that has been employed to model a variety of different real problems in chemistry, physics and biology. Here we study the dynamics of diffusing particles in a domain with an oscillating bubble. Laboratory experiments provide evidence of a non monotone behavior in time of the concentration of particles by a detector located behind the bubble, under suitable experimental condition. A comprehensive explanation of the phenomenon is not yet fully available. The particles are attracted and trapped near the surface of the bubble. The basic mathematical model is a drift-diffusion model, where the particles diffuse and feel the potential of the bubble when they are near its surface. A tentative explanation of the mechanism is based on two-carrier dynamics. The numerical simulation of the system presents two multi-scale challenges. One is spatial: the range of the bubble potential is confined within a few microns at the bubble surface, while the bubble radius is of the order of a millimeter, so a fully resolved solution would be too expensive. The second challenge is on the time scale: the bubble oscillates with a frequency of the order of 100 Hz, while the diffusion time scale is of the order of 1000 seconds, this requiring at least one million time steps to fully resolve the problem in time. A reduced model is derived to solve the multi-scale problem in space for the single carrier dynamics: the interaction with the bubble is modeled as a very thin layer, with a particle surface density proportional to the local density in the bulk, near the bubble. In the rest of the domain the particle density satisfies just a diffusion equation, with suitable boundary conditions on the bubble, deduced from conservation properties. The model is carefully tested on problems in 1D, 2D planar and 3D axis-symmetric geometry. The equation is discretized on a regular Cartesian mesh, using a ghost-point approach, and solved by Crank-Nicolson scheme. The implicit step is efficiently solved by a suitably adapted multi-grid method. The amplitude of the bubble oscillations is small compared to the bubble radius. We take advantage of this fact by replacing the time dependent position by a suitable time dependent velocity at the bubble surface. Because of the low Reynolds number, the velocity distribution is computed by Stokes approximation. The multi-scale challenge in time, as well as the multi-scale model for multi-carrier dynamics are still under investigation.

Chiara Segala  
Università di Trento

*Mean field feedback stabilization of collective behavior*

In the recent years there has been an increasing interest in the study of collective behaviors from the kinetic modelling perspective. In this work we study the control of high-dimensional systems of interacting agents towards a desired configuration. In order to tame the curse of dimensionality, we synthesize feedback controls through the linearization

of the interaction kernel and the solution of a Riccati equation. Hence we propose a feedforward and a feedback approaches to embed the control into the non-linear dynamics. For both approaches we derive a mean-field limit for the constrained microscopic dynamics retrieving a non linear transport PDE coupled with an ODEs for the realization of the feedback. To better understand the control influence we retrieve upper and lower bounds for the decay of the mean-field density towards the desired configuration. Finally, performing a forward error analysis on these bound estimates, we developed a novel numerical method capable to treat efficiently the original high-dimensional control problem, also in the case of limited accessibility to the state of the non linear system. We validate our theoretical results via numerical experiments, showing different applications in the context of opinion formation and alignment dynamics.

Matteo Semplice  
Università dell'Insubria

*1.5D modelling and numerics for shallow water simulations in natural channels*

In this seminar I will consider a "1.5D" model for free-flow in a channel. The channel is represented as a one-dimensional object, but we take into account an arbitrary cross-section at each point along the channel. The model is a one-dimensional hyperbolic balance law with nonconservative products in the source terms; it has always been considered in the literature in a rather involved formulation with source terms depending on the moments of the function describing the cross section and of its derivative along the channel. In the paper by Gouta and Maurel (Int. J. Numer. Meth. Fluid, 2002) where the model was derived, however there is also another much simpler formulation in which the source terms depend only on the free-surface height. In turn, this formulation, together with the path conservative approach, allows the construction of much simpler numerical schemes that are well-balanced, treat correctly the wet-dry transitions and can have arbitrary high order of accuracy. In particular I will discuss finite volume numerical schemes of order up to three, based on the CWENO reconstruction. (Joint work with M. Castro and C. Escalante)

Silvia Tozza  
Università di Napoli Federico II

*A High-Order Scheme for Image Segmentation via a modified Level-Set method*

In this talk I will introduce a high-order accurate scheme for image segmentation based on the level-set method. In this approach, the curve evolution is described as the 0-level set of a representation function but we modified the velocity that drives the curve to the boundary of the object in order to obtain a new velocity with additional properties that are extremely useful to develop a more stable high-order approximation with a small additional cost. We discretize the evolutive problem using a 2D version of a new adaptive filtered scheme for Hamilton-Jacobi equations recently introduced and analyzed in 1D. This approach is interesting since the implementation of the filtered scheme is rather efficient and easy. The scheme combines two building blocks (a monotone scheme and a high-order scheme) via a filter function and smoothness indicators that allow to detect the regularity of the approximate solution adapting the scheme in an automatic way. Numerical tests on synthetic and real images will show the effectiveness of the proposed method and the advantages given by the new velocity. Joint work with Maurizio Falcone and Giulio Paolucci.

Seok-Bae Yun

Sungkyunkwan University, Korea

*Stationary Flows of the ES-BGK model with the correct Prandtl number*

Ellipsoidal BGK model is a general version of the BGK model where the local Maxwellian is generalized to a ellipsoidal Gaussian with a Prandtl parameter  $\nu$  so that the model can produce the correct transport coefficient in the Navier-Stokes limit. In this work, we consider the existence and uniqueness of stationary solutions for ES-BGK model in a slab imposed with the mixed boundary conditions. One of the key difficulties arise in the uniform control of the temperature tensor from below. In the non-critical case  $-1/2 < \nu < 1$ , we utilize the property that the temperature tensor is equivalent to the temperature in this range. In the critical case,  $\nu = -1/2$ , where such equivalence relation breaks down, we observe that the size of bulk velocity in  $x$  direction can be controlled by the discrepancy of boundary flux, to bound the temperature tensor from below. This is a joint work with Stephane Brull.

**Lista Partecipanti** A. Thomann (dottoranda, Università Insubria), G. Naldi (PO, Università di Milano Statale), M. Briani (R, CNR-IAC), E. Cristiani (R, CNR-IAC), Y. Cho (postdoc, Università di Catania), W. Boscheri (R, Università di Ferrara), S.-B. Yun (postdoc, Sungkyunkwan University, Corea), G. Dimarco (PA, Università di Ferrara), L. Bonaventura (PA, Politecnico di Milano), S. Boscarino (PA, Università di Catania), E. Travaglia (dottoranda, Università di Torino), R. Ferretti (PA, Università Roma Tre), M. Falcone (PO, Università Roma Sapienza), L. Saluzzi (dottorando, GSSI L'Aquila), A. Pesare (dottorando, Università di Roma Sapienza), C. Astuto (dottoranda, Università di Catania), C. Segala (dottoranda, Università di Trento), T. Benacchio (postdoc, Politecnico di Milano), L. Pareschi (PO, Università di Ferrara), G. Albi (R, Università di Verona), M. Dumbser (PO, Università di Trento), G. Russo (PO, Università di Catania), M. Semplice (PA, Università di Torino), C. Bassi (postdoc, Politecnico di Milano), S. Busto Ulloa (dottoranda, Università di Trento), E. Macca (dottorando, Università di Catania), G. Puppo (PO, Università di Roma Sapienza), S. Cacace (R, Università Roma Tre), S. Tozza (R, Università di Napoli "Federico II"), E. Iacomini (dottoranda, Università di Roma Sapienza), E. Calzola (dottoranda, Università di Roma Sapienza), G. Paolucci (postdoc, Università di Roma Sapienza), E. Carlini (PA, Università di Roma Sapienza)