Second Year PhD report

Università degli Studi dell'Insubria - Cycle XXXIII

Andrea Thomann
Marie Skłodowska-Curie fellow of the
Istituto Nazionale di Alta Matematica Francesco Severi

Supervisor: Prof. Gabriella Puppo

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1 Attended Activities

1.1 PhD courses

1. *An introduction to networks* (Francesca Arrigo): Introduction to network science and graph theory, centrality measures and their connection to numerical linear algebra
2. *Generalized Locally Toeplitz Sequences: A Spectral Analysis Tool for Discretized Differential Equations* (Carlo Garoni): Introduction to GLT sequences, applications on different discretizations of Convection-Diffusion-Reaction equations in 1D
3. *Reconstruction methods for sparse-data tomography* (Samuli Siltanen): Introduction to sparse-data tomography, measurement and reconstruction of data, programming in Matlab
4. *Statistical Learning Theory and Applications*(Lorenzo Rosasco, Silvia Villa): Introduction to Machine Learning, regularization theory, statistical learning
5. *Fractional diffusion equations: spectral study and design of fast iterative solvers* (Mariarosa Mazza): Study of FDEs from the perspective of GLT sequences, preconditioning, introduction to multigrid methods

1.2 Schools/Workshops

1. Summer School on *Intensive Program on Fluids an Waves: Numerics for Fluids and waves*, Gran Sasso Science Institute (GSSI), L'Aquila, May 21-25 2018.
   Courses: Review on Well-balanced schemes and path-conservative numerical methods (Manuel Castro), Fluids and waves error: control and adaptivity in computational partial differential equations (Omar Lakkis)
2. Workshop on *GPGPU-Computing* (General Purpose Computation in Graphics Processing Unit), Universität Würzburg, October 17-19 2018.

3. CINECA course on *Introduction to Parallel computing using OpenMP and MPI*, Milano, November 12-14 2018.

4. Autumn School on *From interacting particle systems to kinetic equations*, University of Verona, November 26 - 30 2018.
   Courses: Agent Models of 1st and 2nd order: From micro to macro (J.A. Carillo), Mean-field optimal control and other types of games (M. Fornasier), Numerical methods for kinetic and macroscopic equations (L. Wang)

1.3 Conferences

1. *Numerical Aspects of Hyperbolic Balance Laws and Related Problems*, Ferrara, April 16-20 2018.

2. Giornata INdAM, Ferrara, April 18 2018: *Recent advances in multiscale modelling and numerics for hyperbolic and kinetic equations* - in honour of the 60th birthday of Prof. Giovanni Russo.

3. *Tiger-SHARK-FV Conference - Sharing Higher-order Advanced Research Know-how on Finite Volume*, Minho, Portugal, May 20-24 2019.

4. *NumHyp 2019 - Numerical Methods for Hyperbolic Problems*, Málaga, Spain, June 17-21 2019.

1.4 Attended seminars

First year

1. *An all-speed scheme for the simulation of compressible flows and multi-material interfaces*, Emanuela Abbate, Universitá degli Studi dell'Insubria, February, 2018.

2. *From Brownian to pedestrian motion and Fokker-Planck Nash games* Alfio Borzì, Universität Würzburg, May, 2018.

3. *Hidden structures of stochastic numerical methods*, Raffaele D'Ambrosio, Universitá degli Studi dell'Aquila, Italy, May 2018.

4. *Well-posedness of a fluid-particle interaction model*, Jens Klotzky, Universität Würzburg, 2018.

5. *Solar astronomical imaging*, Michele Piana, Universitá di Genova, June 18, 2018.

6. *Coercivity estimates for kinetic equations*, Marlies Pirner, Universität Würzburg, 2018.

7. *High order Finite Volume Schemes for Balance Laws with Stiff Sources*, Matteo Semplice, Universitá degli Studi di Torino, 2018.

Second year

1. *Convegno: Bufale, fake-news, rumors e post-verità: discipline a confronto*, Universitá degli Studi dell'Insubria, February 7, 2019.

2. *General construction of spectra*, Axel Osmond, Université Paris Diderot, May 14, 2019.

3. *A Novel Optimization Approach to Fictitious Domain Methods*, Patrick Guidotti, University of California, July 3, 2019.

4. *The optimal convergence rate of monotone schemes for conservation laws in the Wasserstein distance*, Adrian Ruf, University of Oslo, July 30, 2019.

5. *An accurate front capturing scheme for tumor growth models with a free boundary limit*, Min Tang, Shanghai Jiao Tong University China, August 13, 2019.

2 Passed Exams

First year

1. Exam passed about networks including theory and numerical experiments of exponential and resolvent based centralities (based on the Ph.D course *An Introduction to networks*)

2. Exam passed about the theory of well-balanced higher order path conservative schemes for hyperbolic non-conservative systems (based on the course of M. Castro held at the summer school organised by GSSI)

Second year

3. Exam passed about parallel programming (based on the course *Introduction to Parallel Computing with MPI and OpenMP* organised by CINECA)

4. Exam passed about optimal control of multi particle systems (based on the Autumn school held at the University of Verona)

5. IELTS English Language test (International English Language Testing System), score C1.

3 Publications

Articles

[1] Journal paper: A. Thomann, M. Zenk, C. Klingenberg, *A second-order positivity-preserving well-balanced finite volume scheme for euler equations with gravity for arbitrary hydrostatic equilibria*, International Journal for Numerical Methods in Fluids, 89(11):465–482, 2019.

[2] Journal paper: A. Thomann, G. Puppo, M. Zenk, C. Klingenberg, *An all speed second order IMEX relaxation scheme for the Euler equations*, Communications in Computational Physics, under revision, 2019, preprint on ArXiv.

[3] Journal paper: A. Thomann, G. Puppo, *An all speed second order IMEX relaxation scheme for the Euler equations with gravitional source term*, in preparation, 2019.

[4] Proceedings paper NumHyp 2019: V. Michel-Dansac, A. Thomann, *On high-accuracy L^∞-stable IMEX schemes for scalar hyperbolic multi-scale equations*, submitted, 2019, preprint on HAL.

Talks and Poster presentations

1. Talk: *A second order positivity preserving well-balanced finite volume scheme for Euler equations with gravity*, Autumn school organised by the University of Verona, Italy, (15 min).
2. Talk: *An IMEX FV Scheme for the Euler equations in the low Mach regime*, SHARK-FV Conference, Minho, Portugal, (45 min).
3. Talk: *On finite volume relaxation schemes in the low Mach regime*, Seminar during the research visit to the University of Würzburg, chair of mathematical fluid dynamics, August 2019, Germany, (30 min).
4. Poster presentation: *Second order well-balanced relaxation method for the Euler equations with gravity for hydrostatic equilibria*, Numerical Aspects of Hyperbolic Balance Laws and Related Problems 2018, Ferrara, Italy.
5. Poster presentation: *An IMEX FV Relaxation Scheme for the Euler equations in the low Mach regime*, NumHyp Conference 2019, Málaga, Spain.

4 Research

4.1 Completed projects

Well-balanced scheme for the Euler equations with gravitational source term We study the compressible Euler equations with a gravitational source term. We focus on schemes that can maintain arbitrary hydrostatic equilibria. This are stationary states with zero velocity that balance the pressure gradient and source term exactly. This is achieved by introducing functions α, β that store the reference atmosphere defined by the density and pressure stratification, respectively. The scheme presented in [1] is based on a Suliciu relaxation model which results in a simple wave structure and therefore simplifies the construction of a Riemann solver. The use of the Riemann solver provably guarantees the positivity of density and internal energy which is required for physical applications. We started providing a first order Godunov-type finite volume scheme for the explicit part. Next, we also provided a second order extension of the scheme. Our approach is based on reconstructing equilibrium variables at interfaces which ensures that the well-balanced property is also achieved for the second-order scheme. Since the extension is a convex-combination of first order schemes, it also has the positivity properties.

The project also includes the implementation and testing the properties of the scheme up to three dimensions, i.e. maintaining hydrostatic equilibria on machine precision, designing test-cases for monitoring convergence, Rayleigh Taylor instabilities and strong rarefraction tests.

This is joint work with Markus Zenk & Christian Klingenberg (both Würzburg University).

An all speed scheme for the non-dimensional Euler equations We study the non-dimensional Euler equations. The difference to the aforementioned Euler equations is the appearance of the so called Mach number M due to the scaling process. The Mach number indicates the speed of the gas velocity with respect to the speed of sound and influences drastically the behaviour of the flow. Compressible flows are characterized by high Mach numbers whereas the flow becomes incompressible as $M \to 0$. In [2] we present a scheme that is able to mimic the transition between compressible and incompressible regimes and whose numerical diffusion is provably independent of the choice of the Mach number. This property is essential to maintain the correct transition also at the discrete level. It is known as asymptotic preserving (AP) property. Small Mach numbers are also numerically challenging since they introduce a stiffness into the equations. Therefore we use an implicit-explicit (IMEX) approach to treat the stiff parts of the flux function associated with fast wave speeds implicit and the remaining terms explicit. The scheme is based on a Suliciu type relaxation model which has only contact discontinuities simplifying the construction of the Riemann solver. The explicit part is discretized with a Godunov type finite volume scheme, whereas the implicit part is based on centred differences. In addition to the AP property we can show the positivity of density and internal energy. For the first order IMEX scheme we give a second order extension that inherits the properties of the first order scheme.

The project also includes the implementation and testing of the numerical scheme up to two dimensions. The code includes the PetSc library for solving the implicit system. The performed test-cases in one dimension are a SOD shock tube test and a Mach number dependent shock test to verify that the scheme can capture the correct shock speeds. In two dimensions the Gresho vortex test case is performed which is a stationary solution and is therefore well suited to verify the Mach number independence of the numerical diffusion. To test the second order accuracy, we have introduced a C^1 stationary solution which might become a benchmark test problem to assess the accuracy of low Mach schemes.

This is joint work with Gabriella Puppo (La Sapienza Univ. Rome) & Markus Zenk (Würzburg Univ.).

4.2 Current projects

An all speed scheme for the non-dimensional Euler equations with gravitational source term The aim of this project is to extend the relaxation model and scheme described in [2] with a gravitational source term. Thereby a new parameter, the Froude number Fr, appears from the scaling of the gravitational potential. We are again interested in maintaining stationary states with zero velocity which are, in contrast to the case in [1], depending on the Mach and the Froude number. To have a balance in the limit $M, Fr \to 0$ we focus on the case $\mathcal{O}(M) = \mathcal{O}(Fr)$. For well-balancing the same approach is done as in [1] and it is combined with the IMEX approach. For extension to second order accuracy the reconstruction from [1] is combined with the second order method given in [2]. The numerical order of convergence is verified for the second order scheme in two dimensions. The scheme is expected to be AP in the sense that it maintains well-prepared data and the diffusion is independent of the Mach number. This is already numerically verified through a new Gresho vortex test case that we have adapted to a gravitational potential and might become a benchmark test problem for verifying the Mach number independence of the numerical solution.

The project also includes the study of the positivity of density and internal energy as well as the proof of the AP property. The scheme is implemented up to two dimensions and second order accuracy. Further test cases have to be performed amongst them the rising bubble test case and well-balanced tests.

This is joint work with Gabriella Puppo (La Sapienza University Rome).

IMEX relaxation schemes for hyperbolic multi-scale systems The aim of this project is the extension of the relaxation approach combined with the IMEX splitting used in [2, 3] to general multi-scale systems that are equipped with an equation of state. The objectives are to understand the convergence behaviour and the asymptotic properties of the schemes. We start from a linear ode model characterized by different scales, with tunable eigenvalues, for which we build different operator splitting strategies, in which each scale is treated with a different solver in time. We want to build the scheme in such a way that the order of convergence is preserved across the scales. Afterwards we want to apply the scheme to systems of hyperbolic conservation laws. The expected properties of the scheme include the scale independent time stepping and diffusion.

The project also includes the implementation of the resulting schemes, as well as design and application of suitable test cases to numerically verify the properties.

This is joint work with Gabriella Puppo (La Sapienza University Rome).

High-accuracy L^∞ and TVD stable IMEX schemes for multi-scale problems We study high accuracy L^∞-stable and TVD IMEX schemes for multi-scale problems, characterized by exact solutions satisfying a maximum principle. We study the properties that guarantee that the scheme preserves the maximum principle at the discrete level. These properties can be violated due to oscillations arising mainly from higher order discretizations and the use of central differences in the implicit part. It has been proven that there are only first order IMEX schemes with an upwind discretization that are L^∞-stable and TVD. In [4] the case of a scalar hyperbolic conservation law is investigated for second order IMEX schemes and compared with a MOOD scheme to detect the maximal order of accuracy. The aim of this work is to extend the scheme presented in [4] to systems of conservation laws and to higher order IMEX schemes.

This is joint work with Victor Michel-Dansac (University Toulouse).