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

Organized by
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Abstract. The topic of this workshop was the study of mathematical and numerical analysis for involution-constrained hyperbolic partial differential equations on manifolds. An example is the positivity of the density for the compressible Euler equations. 25 international participants attended the workshop. There were 22 lectures, covering a wide gamut of the topic.

Mathematics Subject Classification (2020): 35L45, 35L65, 58J45, 65M06, 65M08, 65M12, 65M25, 65M60, 74C20, 76W05, 76M12, 78M10, 78M12, 83C05, 83C22.

Introduction by the Organizers

This workshop *Structure-Preserving Discretizations*, organised by Manuel Castro (Malaga), Bruno Després (Paris), Michael Dumbser (Trento) and Christian Klingenberg (Würzburg) was attended by 25 participants with broad geographic representation from all continents. We had 22 lectures, covering the wide gamut of the topic at hand.

In this workshop we discussed progress in mathematical and numerical analysis for involution-constrained hyperbolic partial differential equations on manifolds. Many mathematical models of important physical phenomena are contained in this class of problems, where the involution restricts the space of allowable solutions, such as the well-known condition $\nabla \cdot \mathbf{B} = 0$ in the Maxwell and MHD equations.

While the underlying mathematical theory of many involution-constrained PDEs has been studied, there remain relatively few numerical methods that can preserve the known mathematical structure exactly also on the discrete level.

Examples of topics on structure-preserving schemes are novel well-balanced steady-state preserving methods for conservation laws on manifolds, schemes that respect a discrete entropy inequality, positivity-preserving schemes, as well as Galilean- and rotation-invariant and angular momentum preserving methods on moving meshes.

We had lectures that touched upon various aspects of this subject. Here we list are a few examples. The question on how to properly find time-discretizations in this context was addressed by Philippe Helly, Jean-Luc Guermond and Gabriella Puppo. In lectures by Eric Sonnendrücker, Bruno Despres and Nicolas Crouseille applications to plasma were discussed. Christian Klingenberg, Claudius Birke and Elena Gaburro gave talks on now to maintain stationary solutions. The extended hydrodynamic model by Godunov, Peshkov and Romensky was discussed by Michael Dumbser, Ilya Peshkov and Sergie Gavriluk.

Overall this workshop gave space to discuss the above circle of ideas in the wonderful atmosphere of Oberwolfach.

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

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Abstracts

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

Yann Brenier

1. The isothermal potential Euler equations

The isothermal Euler equations for a gas with density $\rho = \exp(\phi)$, potential velocity $v = \nabla\theta$ and constant speed of sound c read

$$\partial_t v + \nabla(|v|^2/2) + c^2\nabla\phi = 0, \quad \partial_t\phi + v\cdot\nabla\phi + \nabla\cdot v = 0. \tag{1}$$

We may introduce $G = \nabla\phi$ and get the alternative system

$$\partial_t v + \nabla(\frac{|v|^2}{2}) + c^2 G = 0, \quad \partial_t G + \nabla(v\cdot G + \nabla\cdot v) = 0, \tag{2}$$

which is quadratic and preserves the potential character of v and G. Let us introduce the Lagrangian associated with the weak formulation of (2):

$$\mathcal{L} = \int -\partial_t A\cdot v - (\nabla\cdot A)\frac{|v|^2}{2} + c^2 A\cdot G - \partial_t C\cdot G - (\nabla\cdot C)v\cdot G + \nabla(\nabla\cdot C)\cdot v.$$

Differentiating in v and G, we get

$$-\partial_t A - (\nabla\cdot A)v - (\nabla\cdot C)G + \nabla(\nabla\cdot C) = 0, \quad c^2 A - \partial_t C - (\nabla\cdot C)v = 0.$$

Eliminating the t derivatives in $\mathcal{L}$ thanks to these equations, we get the new Lagrangian

$$\mathcal{L}_2 = \int (\nabla\cdot A)\frac{|v|^2}{2} + (\nabla\cdot C)v\cdot G.$$

It is convenient to set $r = \nabla\cdot A$ and $s = \nabla\cdot C$ for which we get

$$\mathcal{L}_2 = \int r\frac{|v|^2}{2} + sv\cdot G, \tag{3}$$

$$\partial_t r + \nabla\cdot(rv) + \nabla\cdot(sG) = \Delta s, \quad \partial_t s + \nabla\cdot(sv) = c^2 r. \tag{4}$$

Let us consider the variational principle of finding the critical points (v, G, s, r) of (3) subject to (4). Introducing α and β as Lagrange multipliers, we get the Lagrangian

$$\int r\frac{|v|^2}{2} + sv\cdot G - \partial_t\alpha r - \nabla\alpha\cdot(rv + sG) - s\Delta\alpha - \partial_t\beta s - \nabla\beta\cdot(sv) - c^2\beta r$$

and get as optimality equations

$$rv + sG - r\nabla\alpha - s\nabla\beta = 0, \quad sv - s\nabla\alpha = 0,$$

$$\frac{|v|^2}{2} - \partial_t\alpha - \nabla\alpha\cdot v - c^2\beta = 0, \quad v\cdot G - \nabla\alpha\cdot G - \Delta\alpha - \partial_t\beta - \nabla\beta\cdot v = 0.$$

Assuming $s \neq 0$, we get

$$v = \nabla\alpha, \quad G = \nabla\beta, \quad -\frac{|v|^2}{2} - \partial_t\alpha - c^2\beta = 0, \quad -\Delta\alpha - \partial_t\beta - \nabla\beta \cdot v = 0,$$

and by setting $\alpha = \theta$, $\beta = \log\rho$ we recover (1). So, we conclude that the isothermal potential Euler equations (1) can be derived from the variational principle (3,4).

2. The free Schrödinger equation

Using the Madelung transform $\psi(t,x) = \sqrt{\rho(t,x)}\,\exp(i\theta(t,x))$, and setting $v = \nabla\theta$, $G = \nabla\log\rho$, the free Schrödinger equation in suitable units reads

$$\partial_t v + \nabla(\frac{|v|^2 - |G|^2}{2}) = \nabla(\nabla\cdot G), \quad \partial_t G + \nabla(v\cdot G) = -\nabla(\nabla\cdot v). \tag{5}$$

Using the same method as for the isothermal potential Euler equations, we get for the free Schrödinger equation

$$\mathcal{L}_2 = \int \frac{|v|^2 - |G|^2}{2} r + sv\cdot G \tag{6}$$

under constraint

$$\partial_t r + \nabla\cdot(rv - sG) = -\Delta s, \quad \partial_t s + \nabla\cdot(sv + rG) = \Delta r, \tag{7}$$

i.e., in complex notations $C = r + is \in \mathbb{C}$, $\quad V_k = v_k + iG_k \in \mathbb{C}$, pour $k \in \{1,\cdots,d\}$,

$$\mathcal{L}_2 = \int \mathcal{R}e(\sum_{k=1}^{d} CV_k^2), \ \text{ s.t. } \ \partial_t C + \sum_{k=1}^{d} \partial_k(CV_k) = i\Delta C.$$

3. The Einstein equations in vacuum with a cosmological constant

A solution to the Einstein equations in vacuum with cosmological constant Λ is defined as a Lorentzian metric g whose Ricci curvature is equal to Λg. By setting

$$V_i^k(x,\xi) = -\Gamma_{ij}^k(x)\xi^j, \quad \Phi(x,\xi) = \log\det g(x) + \frac{1}{2} g_{ij}\xi^i\xi^j, \ \ (x,\xi) \in \mathbb{R}^4 \times \mathbb{R}^4,$$

where Γ_{ij}^k denote the Christoffel symbols, this may be expressed by the system

$$\partial_{x^k} V_j^k + \partial_{\xi^j}(V_k^q V_q^k) - \partial_{x^j} V_k^k - \partial_{\xi^k}(V_j^q V_q^k) + \Lambda\partial_{\xi^j}\Phi = 0,$$

$$\partial_{x^j}\Phi + V_j^m \partial_{\xi^m}\Phi + \partial_{\xi^j} V_m^m = 0,$$

which is striking similar to the isothermal Euler equations (1), where $(x,\xi) \in \mathbb{R}^4 \times \mathbb{R}^4$ substitutes for $(t,x) \in \mathbb{R}\times\mathbb{R}^3$ while Φ, V and Λ substitute for ϕ, v and c^2. Then we may perform (in a work in progress with Philippe Anjolras) the same analysis for the Einstein equations as the one we have just done for the Euler and Schrödinger equations. In the special case of a null cosmological constant (i.e. $\Lambda = 0$), we already obtained in [1]:

Theorem 1. *Let g be a Lorentzian metric on $\mathbb{R}^4$ of zero Ricci curvature and set*

$$A^j(x,\xi) = \xi^j \ \det g(x) \ \cos(\frac{g_{\alpha\beta}(x)\xi^\alpha\xi^\beta}{2}), \quad V_k^j(x,\xi) = -\Gamma^j_{k\gamma}(x)\xi^\gamma,$$

$$C_k^j(x,\xi) = \partial_{\xi^k} A^j(x,\xi) - \partial_{\xi^q} A^q(x,\xi)\ \delta_k^j, \quad (x,\xi)\in\mathbb{R}^4\times\mathbb{R}^4.$$

Then (C,V) is a critical point (with respect to compactly supported perturbations) of

$$\int \mathrm{trace}(C(x,\xi)V^2(x,\xi))dxd\xi = \int (V_\gamma^k C_\sigma^\gamma V_k^\sigma)(x,\xi)dxd\xi,$$

subject to

$$\partial_{x^j} C_k^j + \partial_{\xi^j}(CV+VC)_k^j = 0,$$

$$\partial_{\xi^i} V_j^k = \partial_{\xi^j} V_i^k, \quad 3\partial_{\xi^m} C_k^j - \partial_{\xi^m} C_\gamma^\gamma\ \delta_k^j = 3\partial_{\xi^k} C_m^j - \partial_{\xi^k} C_\gamma^\gamma\ \delta_m^j.$$

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High-order well-balanced implicit and semi-implicit finite-volume methods for systems of balance laws

Manuel J. Castro Díaz

(joint work with Sebastiano Boscarino, Irene Gómez-Bueno, Carlos Parés and Giovanni Russo)

Several physical systems are described by hyperbolic balance laws of the form

$$U_t + F(U)_x = \frac{1}{\epsilon}S(U), \tag{1}$$

where $U(x,t)\in\mathbb{R}^M$ and the right hand side may contain a stiff relaxation source term as the parameter ϵ becomes small. Such systems are efficiently solved by implicit-explicit schemes (IMEX) [1, 8, 2], which treat explicitly the non-stiff hyperbolic term, and implicitly the stiff source term. If S is a relaxation, this means that as $\epsilon\to 0$ the system formally relaxes to conservation law

$$u_t + f(u)_x = 0, \tag{2}$$

where $u(x,t) = QU(x,t)\in\mathbb{R}^m$, $m<M$, $Q\in\mathbb{R}^{m\times M}$, $QS(U)=0 \Leftrightarrow U = E(u)$, $f = QF(E(u))$, which means that the original $M\times M$ hyperbolic system of balance laws relaxes to a $m\times m$ hyperbolic system of conservation laws as the relaxation parameter vanishes (see [5, 6]).

A scheme for the numerical solution of system (1) which becomes a consistent scheme for system (2) as the relaxation parameter vanishes is said to be *Asymptotic Preserving (AP)* (see for example [7, 8]).

If the source term contains a stiff relaxation and a non-stiff term, i.e. a system of the form

$$U_t + F(U)_x = \frac{1}{\epsilon} S(U) + G(U, x), \tag{3}$$

in the limit of vanishing ϵ relaxes to a lower dimensional system of balance laws of the form

$$u_t + f(u)_x = g(u, x), \tag{4}$$

where $g(u, x) = QG(E(u), x)$. In such cases the limit equation admits non-trivial equilibria that must be approximated accurately. Schemes that are able to preserve the non-trivial steady states of system (4) are said to be well-balanced (see [3, 4] and the references therein for a review of the subject).

Now, the goal is to design numerical schemes for system (3) which become consistent and well-balanced schemes for system (4) as the relaxation parameter vanishes, which are said to be *Asymptotic Preserving and Well-Balanced (APWB)*.

Another interesting class of problems appears when both the flux and the source term are (equally) stiff:

$$\epsilon U_t + F(U)_x = G(U, x). \tag{5}$$

In such cases the system may relax to a stationary solution of the ODE system

$$F(U)_x = G(U, x)$$

in a very short time. If one is interested in efficiently capturing the stationary solution, then it is advisable to adopt an implicit (or semi-implicit) scheme which is at the same time well-balanced.

The aim of this talk is to present a general framework to design well-balanced high-order finite volume methods resulting from the combination of the reconstruction technique introduced in [4] and fully implicit or implicit-explicit (IMEX) time integrators introduced in [8, 2], that are suitable for the approximation of problems (3) and (5).

The numerical experiments confirms the good properties of the proposed schemes.

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Quasi-explicit, unconditionally stable, Discontinuous Galerkin solvers for conservation laws

Philippe Helluy
(joint work with Pierre Gerhard, Victor Michel-Dansac)

1. Kinetic approximation of first order conservations laws

In this work, we are interesting in the numerical approximation of a hyperbolic system of m conservation laws in dimension d

$$\partial_t W + \sum_{i=1}^{d} \partial_i Q^i(W) = 0, \tag{1}$$

where the unknown is a vector $W(X,t) \in \mathbb{R}^m$ depending on the space variable: $X = (x_1 \dots x_d)$ and the time variable: t. For the partial derivatives, we use the notation $\partial_i = \frac{\partial}{\partial x_i}$, $\partial_t = \frac{\partial}{\partial t}$.

This kind of system are generally difficult to approximate numerically. One of the difficulties is that explicit schemes are subject to restrictive time steps conditions. Implicit schemes do not suffer from time step conditions but require solving large sets of linear equations. In previous works (see [4] and included references), we have proposed a method, based on a kinetic approach, for avoiding this constraint. We first recall the principles of the kinetic representation.

We consider a set of $d+1$ (or more) kinetic velocities V_k, $k = 0 \dots d$, associated to **vectorial** kinetic functions $F_k(W) \in \mathbb{R}^m$. We also define "Maxwellian" equilibrium functions $M_k(W) \in \mathbb{R}^m$. The kinetic BGK representation is given by transport equations with relaxation source terms [2, 1]

$$\partial_t F_k + V_k \cdot \nabla_X F_k = \frac{1}{\tau} \left(M_k(W) - F_k \right). \tag{2}$$

When the relaxation time $\tau \to 0^+$, the kinetic model (2) is formally equivalent to the initial system of conservation laws (1) provided that

$$W = \sum_k M_k(W), \quad \sum_k V_k^i M_k(W) = Q^i(W), \quad i = 1, \dots, d. \tag{3}$$

Conditions (3) constitute a set of $m(d+1)$ equations with $m(d+1)$ unknowns for finding the Maxwellian. It possesses a unique solution. Theoretical arguments show that the formal limit is a true limit, under a so-called sub-characteristic condition [2, 1]. This condition states that the kinetic velocities have to be greater than the wave speeds λ_r of the underlying hyperbolic system: $\forall k, \quad |V_k| > \max_r |\lambda_r|$.

In practice it is difficult to solve directly the BGK system (2). It is better to split the equations into transport and a collision steps. This leads to the following kinetic algorithm for advancing one time step:

(1) Solve for a duration Δt the free transport equation

$$\partial_t F_k + V_k \cdot \nabla_X F_k = 0.$$

(2) Solve, for the same duration, the relaxation (or collision) step

$$\partial_t F_k = \frac{1}{\tau} \left(M_k(W) - F_k \right).$$

This algorithm is iterated in order to compute an approximation of $W = \sum_k F_k$. The presented splitting algorithm is only first order accurate in time. But it is possible to improve its order, for instance by using an over-relaxation algorithm [4]. It has been observed, since a long time that these kinds of kinetic schemes are free of CFL conditions. See for instance [3]. However, this interesting property is rarely exploited in practical applications.

2. Unconditionally stable DG approximations

The kinetic algorithm presented in Section 1 relies on transport steps and relaxation steps. The relaxation step is generally easy to implement at each interpolation point of the approximation. In addition, it is embarrassingly parallel. The most complicated part of the kinetic algorithm requires solving transport equations of the form

$$\partial_t f + V \cdot \nabla f = 0 \tag{4}$$

If the computational domain has a simple shape and if the solution is computed on a structured Cartesian grid, it is natural to solve this transport equation by the characteristic method. With well-chosen time step Δt and kinetic velocities V_k, this approach leads to the so-called Lattice Boltzmann method.

In a domain Ω with a complex geometry and for unstructured grid, the characteristic method is no more a good choice because it leads to difficulties such as instabilities or loss of conservation. In addition, the treatment of boundary conditions is not natural in this framework. In the unstructured case we prefer to rely on a DG approximation of (4).

We consider an unstructured mesh of the computational domain Ω made of tetrahedral cells. The transported function f is approximated in cell L by a linear expansion on basis functions $f(x,t) \simeq f_L(x,t) = \sum_j f_{L,j}(t)\psi_j^L(x), \quad x \in L$. The unknowns are the coefficients $f_{L,j}(t)$ of the linear expansion. After a DG in space approximation of (4), the DG scheme read as follows

$$\mathbb{K}\mathbb{F}'(t) = 0, \tag{5}$$

where $\mathbb{F}(t)$ is a large vector containing all the coefficients $f_{L,j}(t)$, and $\mathbb{K}$ is the large matrix arising from the DG approximation of the transport equation. We then have to solve a large set of linear Ordinary Differential Equations (ODE).

Explicit-in-time approximations of this set of ODEs suffer from constraining stability conditions on the time step Δt. In order to suppress the stability condition, we can use an implicit time scheme for solving (5) for going from time step $n-1$ to time step n. For simplicity, we describe the case of an implicit first order Euler method. The strategy can be extended to other more accurate schemes, such as the Crank-Nicolson scheme (that we use) or DIRK (Diagonally implicit Runge--Kutta) approaches. With $\mathbb{F}^n \simeq \mathbb{F}(n\Delta t)$, the implicit Euler scheme reads

$$(\mathbb{I} + \Delta t \mathbb{K})\mathbb{F}^{n+1} = \mathbb{F}^n \tag{6}$$

It seems that one would need to assembly and solve a large linear system for computing $\mathbb{F}^{n+1}$ from $\mathbb{F}^n$. But the matrix $\mathbb{K}$ is block-triangular. In practice there is thus an explicit algorithm, the downwind algorithm, for solving efficiently the system (6). See [4].

3. Subdomain parallelism

We have implemented the downwind and the kinetic algorithms in a parallel software based on a work stealing algorithm [4]. We have observed a decreasing efficiency of the method when the number of threads increases. This is because the parallel scaling of the downwind algorithm is limited, at a given point, by the dependencies in the computations.

In order to increase the parallel scaling, we now describe a subdomain strategy that relaxes the computation dependencies. The main idea is to apply the above time-implicit downwind algorithm in each subdomain, but with a time-explicit coupling between the subdomains, for suppressing some dependencies. Because of the explicit coupling, it will be necessary to apply an iterative algorithm for computing the exact solution in a stable way. The algorithm can be proved to converge in a finite number of iterations. In most configurations three iterations are sufficient. Let us now describe the principles of this subdomain iterative algorithm. As in Section 2, the main task is the resolution of the transport equation in $\Omega \times [0, \Delta t]$, with initial data:

$$\partial_t f + V \cdot \nabla f = 0, \quad f(X, 0) = f^0(X).$$

We assume that Ω is decomposed into a finite number of subdomains Ω_i, $i = 1 \dots n_d$. For the simplicity of the presentation, we assume that Ω is a periodic domain or the whole space, in order to avoid the description of the boundary conditions. However the approach is also valid also when $\partial\Omega \neq \emptyset$.

We then denote by f_i the restriction of f to subdomain Ω_i, by $N_i(X)$ the outward normal vector on $\partial\Omega_i$, and by $\partial\Omega_i^-$ the upwind part of the boundary of Ω_i:

$$\partial\Omega_i^- = \{X \in \partial\Omega_i, N_i(X) \cdot V < 0\}.$$

We initialize the algorithm by setting $f_i^0(X, t) = f_i^0(X)$. Thus, the initial iteration does not depend on time. We then consider an iterative algorithm for computing successive time-dependent iterations f_i^p in subdomain Ω_i for $p \geq 1$. For computing

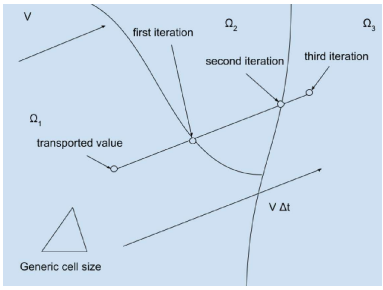

FIGURE 1. Subdomain algorithm, in a generic subdomain decomposition, with corners shared by several subdomains. In this case, the iterative algorithm reaches the exact solution in at most three iterations. First iteration: the boundary value on $\partial\Omega_2^-$ is updated. Second iteration: the boundary value on $\partial\Omega_3^-$ is updated. Third iteration: the correct value is transported.

f_i^p from f_i^{p-1} we solve the following time-dependent boundary value problems

$$\partial_t f_i^p + V \cdot \nabla f_i^p = 0, \quad \text{in } \Omega_i, \tag{7}$$

$$f_i^p(X,0) = f_i^0(X), \quad X \in \Omega_i, \tag{8}$$

$$f_i^p(X,t) = f_j^{p-1}(X,t), \quad X \in \partial\Omega_i^- \cap \partial\Omega_j. \tag{9}$$

We can prove the following result.

Proposition *let L be the maximum diameter of the subdomains. Under the condition*

$$\Delta t \leq \frac{L}{|V|},$$

in the generic case, the above algorithm (7)-(9) converges to the exact solution in at most three iterations: $f_i^3 = f_i$.

The proof relies on the characteristic method. It is briefly sketched in Figure 1.

3.1. **Stability.** We have implemented the above iterative algorithm. The parallelism within each subdomain is managed, as before, through the work stealing strategy. The communications between the subdomains are managed through calls to the MPI (Message Passing Interface) library. In our first experiments, we have verified the stability properties of the transport solver. They indicate that the number of iterations of the iterative algorithm is indeed important for the stability of the method. For a general domain decomposition obtained with an automatic partitioner, and with large time steps, the algorithm is stable provided that three iterations are done for advancing one time step. An illustration is given in Figure 2.

The objective of the subdomain algorithm was to relax the computational dependencies and to achieve a better parallel (strong) scaling of the method.

We compare the time spent in the iterative algorithm with a varying number of threads and subdomains. We define the efficiency e of the acceleration as the

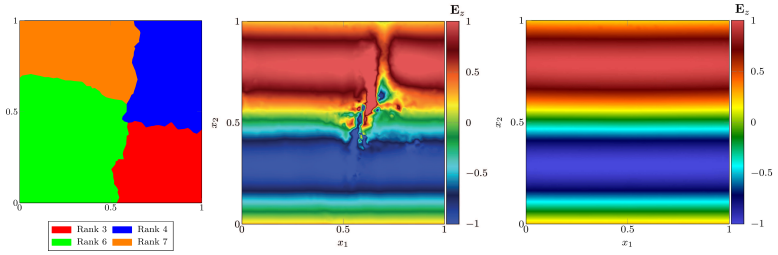

FIGURE 2. Stability of the subdomain iterative algorithm. Left: subdomains structure, Middle: 2 iterations scheme, Right: 3 iterations scheme. We observe that the iterative algorithm is stable, even with large time step, but that three iterations seem to be necessary.

MPI nodes	Threads	#CPU	Time (s)	Accel. e
1	2	2	1314	1
1	8	8	346	0.95
1	**64**	**64**	**106**	**0.39**
2	32	64	75	0.55
8	**8**	**64**	**57**	**0.72**

TABLE 1. Multithread and MPI scaling. For a computation done with 64 threads, we observe that it is better to split the domain into 8 subdomains instead of affecting all the threads to one single subdomain.

ratio of the elapsed time of the algorithm with the time that we would get with an ideal perfect scaling. The efficiency is perfect if $e = 1$. We observe, for instance, that with a single subdomain the efficiency with 64 threads drops to $e = 0.39$, while with 8 subdomains and 8 threads per subdomain the efficiency is better $e = 0.72$. We have thus validated the efficiency of this approach. Of course, the whole algorithm is impacted by a slowdown factor imposed by the additional iterations. However the weak scaling of the method on a supercomputer for very large computations is now certainly ensured. Indeed, explicit subdomain decomposition methods are known to be well adapted to the architecture of supercomputers. More measurements are given in Table 1.

4. Conclusion

We presented an adaptation of the kinetic DG method introduced in [4]. The method can handle arbitrary conservation laws and complex unstructured meshes. It is explicit in time but CFL-free. The method has good parallelization features, for both shared memory and distributed memory computers. For improving the

parallel scaling on distributed memory computers, we have proposed a subdomain decomposition method that relaxes the task dependencies of the kinetic scheme but keeps the possibility to use large time steps.

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Invariant-domain preserving high-order implicit-explicit Runge Kutta time stepping for nonlinear conservation equations

Jean-Luc Guermond
(joint work with Alexandre Ern)

We consider high-order discretizations of the Cauchy problem for a generic conservation equation where the evolution operator comprises a hyperbolic part and a parabolic part with diffusion and stiff relaxation terms. Assuming that the said problem admits an invariant domain, 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 (see [1]), the IMEX scheme is written in incremental form. At each stage of the scheme, we first compute low-order hyperbolic and parabolic updates, then compute the high-order counterparts, and finally apply a conservative limiting technique to the explicit hyperbolic component and to the implicit parabolic part. 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. We propose 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 forthcoming 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 gray radiation.

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Non intrusive low Mach schemes

Gabriella Puppo
(joint work with Andrea Thomann, Angelo Iollo)

In many hyperbolic systems of equations the Jacobian of the system can yield eigenvalues of very different orders of magnitude. One can distinguish *fast* and *slow* waves, and in many applications one is actually interested in slow waves, although the stability restrictions on the time step for explicit schemes are given by the fast waves. The most studied case is in gas dynamics, where the fast scale is given by the acoustic waves, and therefore by the sound speed c, while the slow scale coincides with material waves, and it is given by the actual gas speed, u. Thus the system is stiff when $M = ||u_r||/c_r << 1$ (low Mach flow), where u_r and c_r are reference values for the local velocity of the gas and its sound speed, and their ratio M is the Mach number of the flow.

Low Mach schemes are designed to preserve at the discrete level the asymptotic limit when $M \to 0$, and, at the same time, to avoid the stiffness induced by the low Mach number. The literature in this field is huge, for instance [2, 5] and [3] for an approach based on relaxation. See also the review by [6] and references therein.

Adimensionalizing the equations with respect to the reference values u_r and c_r, the Mach number appears as a parameter. Typical cases are the system of isentropic gas dynamics, which, in adimensional form becomes

$$\partial_t \rho + \nabla \cdot \rho u = 0$$
$$\partial_t \rho u + \nabla \rho u \otimes u + \frac{1}{M^2} \nabla p = 0, \quad p(\rho) = c\rho^\gamma.$$

In a low Mach discretization, the pressure is treated implicitly, thus a typical time discretization takes the form, [8]

$$\rho^{n+1} = \rho^n - \Delta t \, \nabla \cdot (\rho u)^{n+1}$$
$$(\rho u)^{n+1} = (\rho u)^n - \Delta t \nabla (\rho u \otimes u)^n - \Delta t \nabla \left(\frac{1}{M^2} p^{n+1} \right).$$

Then, one substitutes the expression for momentum $(\rho u)^{n+1}$ in the density equation, and, using the fact that the pressure is a known function of the density, the update of the continuity equation becomes an elliptic equation for the density.

The strategy is different if we include the energy equation. The adimensional form of the equations is

$$\partial_t \rho + \nabla \cdot \rho u = 0$$
$$\partial_t \rho u + \nabla \rho u \otimes u + \frac{1}{M^2} \nabla p = 0, \quad p(\rho) = (\gamma - 1)\rho e$$
$$\partial_t E + \nabla (u(E + p)) = 0,$$

but now the dependence on the Mach number appears also in the expression of the energy $E = \frac{1}{\gamma - 1} p + M^2 \rho ||u||^2$. Again, the pressure will be treated implicitly,

and a possible strategy for the time discretization is [4]

$$\begin{aligned}\rho^{n+1} &= \rho^n - \Delta t\ \nabla\cdot(\rho u)^{n+1}\\ (\rho u)^{n+1} &= (\rho u)^n - \Delta t\nabla(\rho u\otimes u)^n + \Delta t\frac{\gamma-1}{2}\nabla(\rho||u||^2)^n - \Delta t\frac{\gamma-1}{M^2}\nabla E^{n+1}\\ E^{n+1} &= E^n + \Delta t M^2\frac{\gamma-1}{2}\nabla(\rho u||u||^2)^n - \Delta t\,\gamma\nabla\left((\rho u)^{n+1}\frac{E^n}{\rho^n}\right)\end{aligned}$$

This time the momentum update is substituted in the energy equation, and the elliptic equation to be solved for the low Mach scheme is in the energy.

We see therefore that the structure of low Mach schemes is typically *intrusive*, in the sense that the design of the scheme is tailored to the structure of the system of equations. An innovative approach could be to provide a general scheme which depends weakly on the structure of the equations. We proposed a general strategy in [10]. The idea is to rewrite the system as a relaxation system, as in [7], thus

$$\begin{aligned}\partial_t u + \partial_x v &= 0,\\ \partial_t v + A^2\partial_x u &= \frac{1}{\eta}(f(u)-v),\end{aligned}$$

where v are relaxation variables, $A^2>0$ is a diagonal matrix of relaxation speeds such that $A^2 > [f'(u)]^2\,\forall u$, and $\eta>0$ is the relaxation rate. In [1], we used this approach, with a fully implicit scheme, to obtain an asymptotic preserving scheme for a multiscale model for elasto-plastic materials. There, we proved that the resulting scheme is AP, provided $\eta < M^2$. The drawback however is that one must also update the relaxation variables. Now, we are proposing a new strategy [10], where the relaxation system is split into a relaxation and a transport step. Namely, we first solve

$$\begin{aligned}\partial_t u &= 0\\ \partial_t v &= \frac{1}{\eta}(f(u)-v).\end{aligned}$$

In the limit $\eta\to 0$, which is the regime of interest, this means immediate relaxation, thus $v^* = f(u^*)$. Then, the convective step starts with initial data $u^n, v^n = f(u^n)$, and is decoupled componentwise,

$$\begin{aligned}\partial_t u_i &= -\partial_x v_i\\ \partial_t v_i &= -A^2\partial_x u_i.\end{aligned}$$

Integrating this system implicitly, we find

$$\begin{aligned}u_i^{n+1} &= u_i^n - \partial_x v_i^{n+1}\\ v_i^{n+1} &= v_i^n - A^2\partial_x u^{n+1}.\end{aligned}$$

Substituting the relaxation variables v_i^{n+1} in the first equation, we find the relaxed implicit system

$$\left(\mathcal{I} - (\Delta t)^2A^2\partial_{xx}^2\right)u^{n+1} = u^n - \Delta t\partial_x f(u^n).$$

This system is provably asymptotic preserving, and can be discretized in space to ensure that the artificial diffusion satisfies the low Mach requirements. Note that this approach does not depend on the particular structure of the system being integrated. For a fully implicit scheme for hyperbolic systems in all regimes, see [9].

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Hamiltonian models in plasma physics and their discretisation

Eric Sonnendrücker

Many kinetic and fluid models in plasma physics have been shown to have a non canonical hamiltonian structure when collisional and dissipative effects are neglected. See in particular the review paper [2]. The concept of geometric or structure preserving discretisation of such Hamiltonian systems has been in intensive area of research in the last few years.

The aim of this talk is to review recent work on this topic. In particular for long time scale computations as is the case in magnetic fusion devices like stellarators and tokamaks, the conservation of the structure of the models and the main invariants is essential.

A non canonical hamiltonian system is characterized by a Poisson bracket and a Hamiltonian $\mathcal{H}$, its abstract formulation being

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F}, \mathcal{H}\}$$

for any functional $\mathcal{F}$.

The guiding principle of geometric methods is to discretize the Poisson bracket and the Hamiltonian rather than the partial differential equations resulting from

them. This enables to get a finite dimensional Hamiltonian system, that can then be solved by classical geometric methods for ordinary differential equations. Note however that the discretisation of the Poisson bracket does not automatically lead to a discrete Poisson bracket as the Jacobi identity is often hard to keep. Still even in this case such a discretisation, which is sometimes called quasi-Hamiltonian in the literature, has good properties and enables the exact conservation of some invariants.

When collisional and dissipative effects become important, a degenerate dissipative metric term can be added to the Poisson bracket. This framework is called metriplectic in the plasma physics community and has been introduced in the 1980s. See in particular [1]. Introducing a hamiltonian $\mathcal{H}$ which is conserved and a free energy (or entropy) $\mathcal{S}$ which is dissipated, the metriplectic dynamical system reads

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F}, \mathcal{H}\} - (\mathcal{F}, \mathcal{S})$$

which can also be expressed as

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \mathbb{J}(U)\frac{\delta \mathcal{H}}{\delta U} - \mathbb{K}(U)\frac{\delta \mathcal{S}}{\delta U}$$

with $\mathbb{J}$ a Poisson operator and $\mathbb{K}$ a symmetric semi-definite positive operator, $\mathcal{F}, \mathcal{S}, \mathcal{H}$ functionals of U.

The entropy is preserved by the Poisson bracket and the energy is preserved by the dissipative bracket

$$\{\mathcal{S}, \mathcal{H}\} = 0, \ (\mathcal{H}, \mathcal{S}) = 0.$$

This implies in particular that the energy is preserved and the entropy dissipated:

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}t} = \{\mathcal{H}, \mathcal{H}\} - (\mathcal{H}, \mathcal{S}) = 0, \ \frac{\mathrm{d}\mathcal{S}}{\mathrm{d}t} = \{\mathcal{S}, \mathcal{H}\} - (\mathcal{S}, \mathcal{S}) \leq 0.$$

Our main application of geometric discretisations in the talk is the Vlasov-Maxwell-Landau model. It fits into the metriplectic framework with

$$\frac{\mathrm{d}\mathcal{F}}{\mathrm{d}t} = \{\mathcal{F}, \mathcal{H}\} + (\mathcal{F}, \mathcal{S}),$$

$$\mathcal{H} = \frac{m}{2}\int f v^2 \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v} + \frac{\epsilon_0}{2}\int E^2 \mathrm{d}\mathbf{x} + \frac{1}{2\mu_0}\int B^2 \mathrm{d}\mathbf{x},$$

$$\mathcal{S} = \int f \ln f \mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}.$$

The metriplectic bracket preserves mass, momentum, total energy, the divergence constraints on E and B, and satisfies an H-theorem, implying monotonic dissipation of entropy, and the existence of a unique equilibrium state.

A discretisation of the brackets, the hamiltonian and the entropy, instead of the associated partial differential equations guarantees these properties at the discrete level and can be achieved by different numerical methods. We used in particular Finite Element Exterior Calculus to discretize the fields and a Particle-In-Cell approximation of the Vlasov equation [3]. A generalization of this method has

been described in [5] and an implicit formulation in [4]. A variational stochastic formulation for collisional operators has been derived in [6].

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Vlasov equations (for plasmas) and Friedrichs systems

Bruno Després

(joint work with Frédérique Charles, Ruiyong Dai, Sever Hirstoaga)

This contribution describes the structure of the new anisotropic moment model (12) written at the end of this contribution. The model is under development at the Muffin project (funded by ANR project MUFFIN).

The starting point is a model Vlasov equation with non constant magnetic field

$$\partial_t f + \mathbf{v} \cdot \nabla_x f + (\mathbf{E}(\mathbf{x}) + \mathbf{v} \times \mathbf{B}_0(\mathbf{x})) \cdot \nabla_v f = 0. \tag{1}$$

In this equation $\mathbf{x} \in \mathbb{R}^3$ is the space variable, $\mathbf{v} \in \mathbb{R}^3$ is the velocity variable, $t > 0$ is the time variable and $f = (\mathbf{x}, \mathbf{v}, t)$ is the unknown. The magnetic field is written as

$$\mathbf{B}_0(\mathbf{x}) = \frac{\omega_c(\mathbf{x})}{\varepsilon} \mathbf{b}_0(\mathbf{x})$$

where $|\mathbf{b}_0(\mathbf{x})| = 1$ and the magnitude of the magnetic field is $\frac{\omega_c(\mathbf{x})}{\varepsilon}$ where $\omega_c(\mathbf{x}) > 0$ is the cyclotron frequency and $\varepsilon \in (0, 1]$ allows to study the regime of strong magnetic field $\varepsilon \to 0^+$. We quote that $\nabla_v \cdot (\mathbf{E}(\mathbf{x}) + \mathbf{v} \times \mathbf{B}_0(\mathbf{x})) = 0$.

Recent mathematical results on such models are in [8, 7]. The method of moments for the discretization of kinetic equations for particles in plasma is studied in [1, 2, 3, 4, 6]. Trefftz methods applied to moment models of kinetic equations for neutral particles with scattering an absorption [5] have a similar structure. With respect to these works, the originality of this contribution is the anisotropy brought by the non constant magnetic field. A new expansion is proposed in terms of anisotropic shape functions aligned with the direction of the magnetic direction $\mathbf{b}_0(\mathbf{x})$.

1. Construction of the method

The Hermite functions are well adapted to the Gaussian kernel which describe the underlying statistical equilibrium of a plasma. They are denoted as

$$\varphi_n(v) = (-1)^n (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{\frac{v^2}{2}} \frac{d^n}{dv^n} e^{-v^2} = (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{\frac{-v^2}{2}} H_n(v), \quad n \in \mathbb{N},$$

where $(H_n)_{n\in\mathbb{N}}$ is the family of Hermite polynomials. The first terms in the series are

(2)

$$\varphi_0(v) = \pi^{-\frac{1}{4}} e^{-\frac{v^2}{2}}, \ \varphi_1(v) = \sqrt{2}\pi^{-\frac{1}{4}} v e^{-\frac{v^2}{2}}, \ \varphi_2(v) = \left(\sqrt{2}\pi^{\frac{1}{4}}\right)^{-1} (2v^2 - 1) e^{-\frac{v^2}{2}}.$$

A generating formula is $\varphi_n(v) = (-1)^n (2^n n! \sqrt{\pi})^{-\frac{1}{2}} e^{\frac{v^2}{2}} \frac{d^n}{dv^n} e^{-v^2}$. The Hermite functions form an orthonormal family $\int_{\mathbb{R}} \varphi_m(v)\varphi_n(v)dv = \delta_{mn}$ which is complete in the space of quadratically integrable functions $L^2(\mathbb{R})$. For all g such that $\int_{\mathbb{R}} g^2(v)dv < \infty$, one has the identity in $L^2(\mathbb{R})$

$$g(v) = \sum_{n\in\mathbb{N}} g_n \varphi_n(v)dv \qquad \text{where } g_n = \int_{\mathbb{R}} \varphi_n(v) g(v) dv.$$

Two important formulas are satisfied

$$v\varphi_n(v) = \sqrt{\frac{n+1}{2}}\varphi_{n+1}(v) + \sqrt{\frac{n}{2}}\varphi_{n-1}(v), \quad n \in \mathbb{N}, \tag{3}$$

and

$$\varphi_n'(v) = -\sqrt{\frac{n+1}{2}}\varphi_{n+1}(v) + \sqrt{\frac{n}{2}}\varphi_{n-1}(v), \quad n \in \mathbb{N}. \tag{4}$$

As in [1, 2], it is convenient to define the asymmetric basis $\psi_n(v) = e^{-\frac{v^2}{2}}\varphi_n(v) = (2^n n!\sqrt{\pi})^{\frac{1}{2}} e^{-v^2} H_n(v)$ and $\psi^n(v) = e^{\frac{v^2}{2}}\varphi_n(v) = (2^n n!\sqrt{\pi})^{\frac{1}{2}} H_n(v)$. A generic notation for a multi-index with three components is

$$\mathbf{n} = (n_0, n_1, n_2) \in \mathbb{N}^3 \text{ with } |\mathbf{n}| = n_0 + n_1 + n_2.$$

To be compatible with the notion of physical Maxwellians [1] and to take into account the anisotropy brought by the magnetic field $\mathbf{B}_0(\mathbf{x})$, we rescale the parallel direction

$$\mathbf{d}_0(\mathbf{x}) = \frac{\mathbf{b}_0(\mathbf{x})}{\sqrt{T}} \tag{5}$$

where $T > 0$ is the temperature, assumed to be constant in space and time in this simple modeling. We complete $\mathbf{b}_0(\mathbf{x})$ as a local direct orthonormal basis

$$\mathbf{b}_i(\mathbf{x}) \cdot \mathbf{b}_j(\mathbf{x}) = \delta_{ij}$$

and rescale the orthonormal directions as

$$\mathbf{d}_i(\mathbf{x}) = \frac{\mathbf{b}_i(\mathbf{x})}{\sqrt{T}}, \qquad i = 1, 2. \tag{6}$$

We define

$$\boldsymbol{\varphi}_{\mathbf{n}}(\mathbf{x},\mathbf{v}) = \varphi_{n_0}\left(\mathbf{v}\cdot\mathbf{d}_0(\mathbf{x})\right)\varphi_{n_1}\left(\mathbf{v}\cdot\mathbf{d}_1(\mathbf{x})\right)\varphi_{n_2}\left(\mathbf{v}\cdot\mathbf{d}_2(\mathbf{x})\right), \tag{7}$$

which is an orthonormal and complete family with respect to the velocity variable $\mathbf{v}$ with continuous dependance with respect to the space variable $\mathbf{x}$. The corresponding asymmetric families are

$$\boldsymbol{\psi}_{\mathbf{n}}(\mathbf{x},\mathbf{v}) = \psi_{n_0}\left(\mathbf{v}\cdot\mathbf{d}_0(\mathbf{x})\right)\psi_{n_1}\left(\mathbf{v}\cdot\mathbf{d}_1(\mathbf{x})\right)\psi_{n_2}\left(\mathbf{v}\cdot\mathbf{d}_2(\mathbf{x})\right) \tag{8}$$

and

$$\boldsymbol{\psi}^{\mathbf{n}}(\mathbf{x},\mathbf{v}) = \psi^{n_0}\left(\mathbf{v}\cdot\mathbf{d}_0(\mathbf{x})\right)\psi^{n_1}\left(\mathbf{v}\cdot\mathbf{d}_1(\mathbf{x})\right)\psi^{n_2}\left(\mathbf{v}\cdot\mathbf{d}_2(\mathbf{x})\right) \tag{9}$$

By construction

$$\boldsymbol{\psi}_{\mathbf{n}}(\mathbf{x},\mathbf{v}) = e^{-\frac{|\mathbf{v}|^2}{2T}}\boldsymbol{\varphi}_{\mathbf{n}}(\mathbf{x},\mathbf{v}) \text{ and } \boldsymbol{\psi}^{\mathbf{n}}(\mathbf{x},\mathbf{v}) = e^{\frac{|\mathbf{v}|^2}{2T}}\boldsymbol{\varphi}_{\mathbf{n}}(\mathbf{x},\mathbf{v}). \tag{10}$$

The functions $\psi^{\mathbf{n}}$ with the upper-script $\mathbf{n}$ are polynomials.

The approximation method is based on a finite expansion coupled with many equations

$$\begin{aligned} &f^N(\mathbf{x},\mathbf{v},t) = \textstyle\sum_{|\mathbf{m}|\le N} u_{\mathbf{m}}(\mathbf{x},t)\boldsymbol{\psi}_{\mathbf{m}}(\mathbf{x},\mathbf{v}),\\ &\int_{\mathbf{v}}\left(\partial_t f^N(\mathbf{x},\mathbf{v},t) + \mathbf{v}\cdot\nabla_x f^N(\mathbf{x},\mathbf{v},t) + \mathbf{F}(\mathbf{x},\mathbf{v})\cdot\nabla_v f^N(\mathbf{x},\mathbf{v},t)\right)\boldsymbol{\psi}^{\mathbf{n}}(\mathbf{x},\mathbf{v})dv = 0\\ &\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \forall(\mathbf{x},t) \text{ and } |\mathbf{n}|\le N. \end{aligned} \tag{11}$$

where the force is $\mathbf{F}(\mathbf{x},\mathbf{v}) = \mathbf{E}(\mathbf{x}) + \mathbf{v}\times\mathbf{B}_0(\mathbf{x})$.

2. Structure of the final anisotropic Moment model

Let us decompose $\mathbf{E} = (E_1, E_2, E_3)$. It is easily shown that the moment model (11) is equivalent to the Friedrichs system

$$\partial_t U(\mathbf{x},t) + \sum_{i=1}^{3}\partial_{x_i}\left(A_i(\mathbf{x})U(\mathbf{x},t)\right) - B(\mathbf{x})U(\mathbf{x},t) + C(\mathbf{x})U(\mathbf{x},t) + \sum_{i=1}^{3}E_i(\mathbf{x},t)D_i(\mathbf{x})U = 0 \tag{12}$$

coupled with the Poisson equation. The unknown is the vector of moments $U(\mathbf{x},t)$. The point is that all matrices can be calculated explicitly and that the large magnetic field limit ($\varepsilon\to 0$) is compatible with the recent results [8].

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Comparison of high-order Eulerian methods for electron hybrid model

Nicolas Crouseilles
(joint work with Anais Crestetto, Yingzhe Li, Josselin Massot)

In this work [1], we focus on the numerical approximation of a hybrid fluid-kinetic plasma model for electrons, in which energetic electrons are described by a Vlasov type model whereas a fluid model is used for the cold population of electrons. The two models are coupled through the current in the Maxwell equations for the electromagnetic fields.

First, we study the validity of this hybrid modelling in a two dimensional context (one dimension in space and one dimension in velocity) against the full (stiff) Vlasov model and second, a four dimensional configuration is considered (one dimension in space and three dimensions in velocity) following [3].

To do so, we consider two numerical Eulerian methods. The first one is based on the Hamiltonian structure of the hybrid model which enables us to design Hamiltonian splitting. It turns out that each subsystem of this splitting can be solved exactly in time, and high order methods are used to discretize the phase space. This approach leads to very good conservation of the total energy for large time, but turns out to be very costly when one is interested in high order splittings in the four dimensional case. A second approach is based on exponential integrators [2] where the linear terms of the hybrid model are solved exactly in time. This approach enables to derive high order time integrators still removing the CFL condition induced by the linear part (which is the most stringent one). We also propose a Padé technique to approximate the exponential of the matrix involved in the exponential integrators.

The accuracy and 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.

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Structure preserving numerical methods for the Euler equations with gravity

Christian Klingenberg

This report summarizes some of the work that resulted from the collaboration with the astrophysicist Fritz Röpke (Heidelberg) (click here for Röpke). He does numerical simulations of convection inside a star. At the heart of his PDE model are the compressible Euler equations with gravity:

$$\begin{cases} \partial_t \rho + \nabla_x \cdot (\rho u) = 0 \\ \partial_t \rho u + \nabla_x (\rho u \otimes u + p) = -\rho \nabla \Phi \\ \partial_t E + \nabla_x \left((E + p) u \right) = -u \rho \nabla \Phi, \end{cases}$$

where Φ is a given gravitational potential, ρ the density, u the velocity, $p = p(\rho, e)$ is the pressure, which is a given function of density and internal energy e.

In Röpke's astrophysical applications (see for example [6]) the flow is near a hydrostatic equilibrium and also tends to have very low Mach number. A hydrostatic equilibrium is a stationary solution with zero velocity, the Mach number represents the speed of the flow compared to the sound speed. It can be shown that solutions of the compressible flow equations converge to solutions of the incompressible flow equations, see [7].

This puts two requirements on the numerical scheme for such flows:

- the scheme should maintain a numerical discretization of the hydrostatic equilibrium exactly, called well-balanced
- in the limit to incompressible equations the scheme should also be able to discretize these limit equations.

We shall report on a number of schemes that well-balanced, see e.g. [3], [4], [6].

Numerical schemes that manage to to maintain stationary solutions should also be able follow the low Mach limit. We study schemes that are able to do both. It is important to pay attention to the interplay of these two properties. We shall report on this as presented e.g. in [1], [5], [8].

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

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

Claudius Birke
(joint work with Christophe Chalons, Christian Klingenberg)

In physical applications, problems with large scale differences can occur, so that the Mach number becomes very small. It is commonly known that for such problems standard finite volume schemes suffer from excessive dissipation. This can be explained by analysing the structure of numerical fluxes in finite volume methods. In general, finite volume fluxes consist of a central flux combined with an artificial dissipation term, i.e.

$$\mathbf{F}(\mathbf{U}^L, \mathbf{U}^R) = \frac{1}{2}\left(\mathcal{F}(\mathbf{U}^L) + \mathcal{F}(\mathbf{U}^R)\right) - \frac{1}{2}\mathbf{D}(\mathbf{U}^R - \mathbf{U}^L). \tag{1}$$

This dissipation term, introduced for stability, scales with the largest wave speed of the underlying system. For the compressible Euler equations it therefore scales with the inverse of the Mach number, i.e. $\mathbf{D} \sim \mathcal{O}(1/M)$. In combination with the difference between left and right state of the velocity at the Riemann problem, this leads to a very large dissipation which prevents an accurate resolution of the fluid flow. Based on this problem analysis, low Mach fixes were introduced for various approximate Riemann solvers to reduce dissipation. In low Mach versions of Roe's solver, the dissipation matrix is rescaled by multiplying by carefully chosen preconditioning matrices [1, 2], while in HLL-type solvers it is sufficient to redefine the intermediate state of the pressure [3]. When incorporating this low dissipation strategy into the theory of Suliciu type relaxation solvers [4] as well, the subcharacteristic condition for stability has to be taken into account. Unfortunately, it is not possible to simply rescale the already existing relaxation speed to reduce dissipation, as this would violate the subcharacteristic condition. To circumvent this conflict, Bouchut *et al.* add a second relaxation speed to their relaxation

system for solving the homogeneous barotropic Euler equations [5]. The key idea here is to not only to reduce dissipation on the velocity, but to simultaneously increase dissipation on the density. So, in a way, a transfer of dissipation takes place. As a result, the dissipation remains bounded for low Mach numbers, while the subcharacteristic condition remains fulfilled. The additional dissipation on the density does not result in a reduced accuracy since the density difference scales with M^2 and thus the dissipation remains bounded.

We extend this low Mach approach to the full Euler equations and consider additionally gravitational source terms [6]. In this context one must also consider the influence of the source term on steady solutions. For problems close to hydrostatic equilibrium

$$\begin{cases} \mathbf{u} = 0, \\ \nabla p = -\rho \nabla \Phi, \end{cases} \tag{2}$$

standard finite volume methods do not automatically satisfy a discrete equivalent of (2) and therefore are not capable of resolving small perturbations on the equilibrium accurately on coarse grids. In order to adress this we combine the two-speed system with a well-balancing mechanism that was introduced in [7]. The key idea of this approach is to add a transport relaxation equation for the gravitational potential to the relaxation system in order to include the gravitational potential into the approximate Riemann solver. The additional equation in the relaxation system leads to a Riemann problem that is under-determined, which gives an additional degree of freedom and allows to introduce a closure equation that is a discrete equivalent of (2). This technique makes it possible to preserve all hydrostatic equilibria up to second order accuracy, certain families of equilibria and a-priori known hydrostatic solutions even up to machine precision.

The resulting approximate Riemann solver is proven to be well-balanced and asymptotic preserving. In the asymptotic-preserving proof, it becomes clear that the asymptotic-preserving property is closely related to the well-balanced property. In fact, in addition to the reduced dissipation coming from the Mach number dependent scaling of the relaxation speeds, in the proof it is also exploited that in the low Mach limit the hydrostatic equilibrium is satisfied up to errors of order M^2.

By respecting the subcharacteristic condition, the solver satisfies a discrete version of the entropy inequality, with the help of which it can be proven that no unphysical checkerboard modes can occur in the velocity and the pressure. Additionally, the approximate Riemann solver preserves the positivity of density and internal energy.

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Structure preserving schemes for general relativity

Elena Gaburro
(joint work with Simone Chiocchetti, Manuel Castro and Michael Dumbser)

The aim of the work presented during the seminar is the development of a new family of numerical schemes able to simulate in a robust way and over very long computational times the evolution of both the *matter* and the *metric* of the space time according to the theory of *general relativity*.

To this scope the use of *high order* Finite Difference, Finite Volume (FV) and/or Discontinous Galerkin (DG) schemes represents, unlikely, only the starting point. Indeed, the high order of accuracy is a fundamental ingredient to reduce the numerical errors and provide high accurate schemes, but is not enough to guarantee the robustness. Thus, it is necessary to endow these methods with additional features able to preserve also at the discrete levels many of the physical constraints satisfied by the continuum model.

At this purposes, we have addressed three topics: i) well balanced schemes, i.e. schemes able to preserve the equilibrium solutions of the studied systems up to machine precision, ii) curl cleaning methods able to control the numerical errors affecting variables which at continuum level have provable zero or constant curl, and iii) a new family of direct Arbitrary-Lagrangian-Eulerian schemes allowing to exploit the Galilean and rotational invariance of the system preserving at the same time a high quality of the moving meshes.

Before moving to the details of these structure preserving numerical techniques, it is worthy to provide the *mathematical formulation* of the studies systems, which is given by systems of *first order hyperbolic* partial differential equations.

The evolution of the matter is given by the so called GRMHD system, see for example [5]. This system of 19 equations can be considered alone, in this case the metric is fixed and we are said to work in a so called *Cowling approximation*. The evolution of the metric is given by the FO-CCZ4 Eistein field equations, see for example [4]. This system of 59 equations can be considered alone, in this case the matter is fixed and we are said to work in a so called *anti-Cowling approximation*.

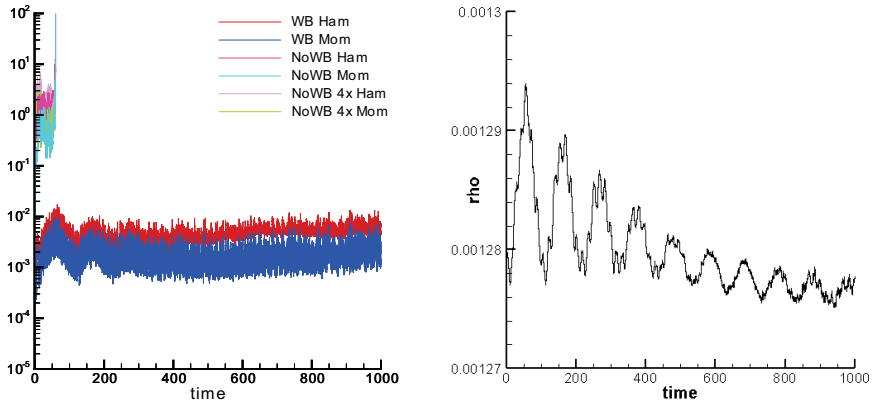

FIGURE 1. TOV star simulation with the CCZ4+GRHD fully coupled model corresponding to an initial perturbation over the pressure profile p. Left: we show the values of the Hamiltonian and momentum constraints which are close to machine precision and constantly maintained for long computational times with the WB code, while they rapidly blow up with the not WB code. Right: we plot the numerical results obtained with the new WB scheme for the density of the star at an inner point with $r = 0.5$ which oscillates due to the initial pressure perturbations.

The two systems can also be considered together: in this case we can study the joint evolution of metric and matter according to general relativity, see for example [1].

However, the coupled system counts many equations with stiff sources and delicate variables quite sensible to numerical errors. To allow its robust and long time simulation we have started with the introduction of well balanced (WB) techniques. The details on the construction of a second order well balanced FV scheme have been given in the talk and can be found in [1]. A remarkable result of this work is that the obtained numerical scheme allowed for the first time in literature to study of the pulsation of a TOV neutron star subject to a pressure perturbation, see Figure 1.

Then, the necessity of techniques able to preserve curl involution, for moving to higher dimension simulations, has been addressed. The focus was put in particular on a novel curl cleaning technique, see [4]. I refer to the talk given by Michael Dumbser and Ilya Peshkov for more details.

Finally, a novel family of high order accurate direct Arbitrary-Lagrangian-Eulerian (ALE) FV and DG schemes over moving Voronoi meshes with topology changes

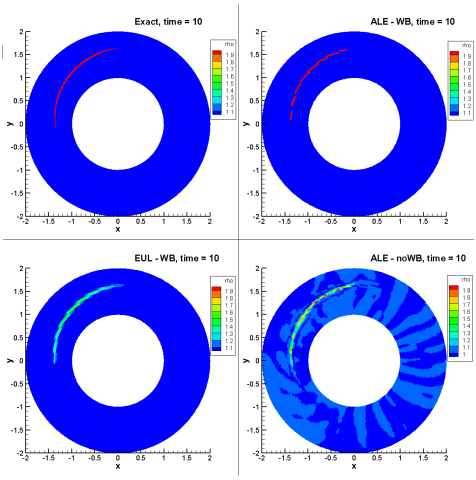

FIGURE 2. We compare the exact solution with the numerical solutions obtained with different methods for a mass transport over a Keplerian disk. For all the cases the employed numerical flux is an Osher-type flux. The Lagrangian algorithms show their ability in reducing the viscosity along the angular direction. The well balanced methods do not diffuse the quantities in the radial direction. When coupled together (top-right) we obtain a result very close to the exact solution (top-left).

has been presented, see [3, 2]. This novel approach, involving high quality of the grid moving in a way as much as possible Lagrangian together with high order of accuracy, offers a robust framework with reduced dissipation errors on convective terms, exceptionally suitable for the treatment of vortical flows around central objects as black holes and neutron stars. Based on previous results of well balancing coupled with direct ALE for simpler equations as Euler with gravity, see [6] and Figure 2, the insertion of well balanced techniques inside this new family of schemes represents a promising framework for further simulation of phenomena involving general relativity.

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Time integration of the semi-discrete Active Flux method

Wasilij Barsukow

Hyperbolic systems of conservation laws are known to develop discontinuities in finite time. At least in one spatial dimension, for systems such as the Euler equations, the behaviour of discontinuities can be computed analytically. In the quest for reliable, i.e. stable and accurate numerical methods for hyperbolic conservation laws, Godunov [7] suggested to interpret the discrete data as a piecewise constant function with jumps at every cell interface, and to update the discrete data by evolving this piecewise constant function exactly over a short period of time. To this end, the Riemann problems at cell interfaces need to be solved, and the time span is chosen such that waves from neighbouring Riemann problems cannot interact. After this time span, the solution is averaged over the cells, i.e. projected again on a piecewise constant function. Godunov's method therefore is a fully explicit method.

One observes that this approach, if applied to the linear advection equation, yields the upwind method. At the same time, for nonlinear equations, the numerical method can become fairly complicated, because the exact solution of the Riemann problem appears as a part of it. At the same time, the usage of the exact solution as a building block allows to prove a discrete entropy inequality easily. Many works have been devoted to a derivation of approximate Riemann solvers, e.g. [8, 5, 9].

If a shock is present in a numerical simulation, it is generally never resolved by a single jump located at a cell interface. In general, it is approximated by several jumps and smeared out over a number of cells. Moreover, smooth parts of the flow, such as rarefactions, are "cut" by Godunov's approach into piecewise constants at every time step.

There exist many suggestions in the literature, how continuous interpretations of discrete data can be constructed. One example are classical Finite Elements. The Galerkin method with test and basis functions that are piecewise linear and globally continuous, however, is unstable for hyperbolic problems if integrated explicitly, as this method can be seen as a finite difference approximation that employs central derivatives, i.e. no upwinding.

The Active Flux method ([10, 6]) chooses a continuous interpretation of the data as well, and allows to achieve stability naturally. Its degrees of freedom are cell averages $\{\bar{q}_i : i \in \mathbb{Z}\}$ and point values $\{q_{i+\frac{1}{2}} : i \in \mathbb{Z}\}$ at cell interfaces. These point values are shared, i.e. the natural interpretation of the discrete data is piecewise parabolic, and globally continuous. The parabola $q_{\mathrm{recon},i} \in P^2([-\frac{\Delta x}{2}, \frac{\Delta x}{2}])$ in cell i fulfills

$$q_{\mathrm{recon},i}\left(\pm\frac{\Delta x}{2}\right) = q_{i\pm\frac{1}{2}} \qquad \frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} \mathrm{d}x\, q_{\mathrm{recon},i}(x) = \bar{q}_i. \tag{1}$$

Following [1], integration of the conservation law $\partial_t q + \partial_x f(q) = 0$ over the cell yields the evolution equation for cell averages:

$$\frac{\mathrm{d}}{\mathrm{d}t}q_i(t) + \frac{f(q_{i+\frac{1}{2}}(t)) - f(q_{i-\frac{1}{2}}(t))}{\Delta x} = 0. \tag{2}$$

This equation is exact; the order of accuracy of the method therefore is determined by the order of accuracy of the point value update and the order of accuracy of the time integration.

The classical update of point values ([10, 2]) is obtained by considering the exact or approximate evolution of the reconstruction. While for linear problems it is possible to use exact evolution operators ([4]), for nonlinear problems this is cumbersome even for smooth solutions. When characteristics cross, in general, extra care is required ([2]). This approach does not yield an ODE for each $q_{i+\frac{1}{2}}(t)$, but determines the value $q_{i+\frac{1}{2}}(\Delta t)$ directly. The usage of characteristic tracing therefore is mixing the spatial differentiation (essentially hidden in the evaluation of the parabola at the foot point of the characteristic) with time integration (which happens in the calculation of where that foot point would be). For linear advection $\partial_t q + c\partial_x q = 0$, $c > 0$, one finds for example

$$q_{i+\frac{1}{2}}^{n+\frac{\ell}{2}} = q_{i+\frac{1}{2}}^{n}\left(1 - 2\lambda\ell + \frac{3}{4}\lambda^2\ell^2\right) + q_{i-\frac{1}{2}}^{n}\left(-\lambda\ell + \frac{3}{4}\lambda^2\ell^2\right) - \frac{3}{2}\lambda\ell\bar{q}_i^n(\lambda\ell - 2) \tag{3}$$

with $\Delta t = \lambda\Delta x/c$. The reason for computing point values for several times is the update of the average, which, upon integration of (2) over the time step $[0, \Delta t]$ requires time-quadratures of fluxes:

$$\frac{\bar{q}_i^{n+1} - \bar{q}_i^n}{\Delta t} + \frac{1}{\Delta t}\int_0^{\Delta t} \mathrm{d}t \frac{f(q_{i+\frac{1}{2}}(t)) - f(q_{i-\frac{1}{2}}(t))}{\Delta x} = 0. \tag{4}$$

These quadratures can easily be obtained via Simpson's rule:

$$\frac{1}{\Delta t}\int_0^{\Delta t} \mathrm{d}t f(q_{i+\frac{1}{2}}(t)) \simeq \frac{1}{6}\left(f(q_{i+\frac{1}{2}}^n) + 4f(q_{i+\frac{1}{2}}^{n+\frac{1}{2}}) + f(q_{i+\frac{1}{2}}^{n+1})\right). \tag{5}$$

This approach therefore is a leap-frog-type time integration: it uses the point values at time $n + 1$ to perform the update of the averages. It is stable up to $\lambda = 1$, i.e. up to the physical stability bound.

In [1] it has also been suggested to write down an ODE for the evolution of the point values. Leaving the time continuous, it thus requires an approximation to the spatial derivative, e.g. as a finite difference formula. The resulting system of ODEs (one for the point values and (4) for the averages) is solved with standard time integrators, such as SSP-RK. Several such suggestions have been presented in the talk. They generally are stable under slightly stricter CFL conditions than the physical one, and the stability depends on the upwinding of the stencil. They come at the advantage that an extension to e.g. nonlinear systems such as the Euler equations is immediate, while the characteristic tracing algorithm depends a lot on whether a scalar conservation law is solved, a system (in 1-d or in multi-d), a homogeneous or an inhomogeneous problem ([3]), etc.

Future work will be devoted to the extension of these results to arbitrary order of accuracy and to multiple spatial dimensions.

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

Barbara Re
(joint work with Rémi Abgrall)

Compressible multiphase flow fields are characterized by the presence of interfaces, which separate two (or more) phases or components, distinguished by different physical or chemical properties. Among the simulation tools specifically developed to deal with them, diffuse-interface methods (DIMs) resort to an augmented system of governing equations to dynamically capture the interfaces. Indeed, rather than explicitly tracking the interface motion, its position is reconstructed from an integral quantity, such as the volume fraction α. Derived through an average process, the governing equations of DIMs include some interfacial terms, which describe the exchange between phases. Among the different closure assumptions proposed to describe the dynamics of immiscible two-phase flows, Baer-Nunziato (BN) type models are the most general ones, which assume that each phase evolves with its own pressure, velocity, and temperature. Despite the complexity arising from the large number of equations, an important advantage of these models is the use of a thermodynamic model for each phase, so there is no need to define an equation of state for the mixture.

In this work, we derive a pressure-based BN-type model able to deal with any equation of state written in the generic form $P = P(e, \rho)$, with P the pressure, e the internal energy per unit of volume, and ρ the density. The proposed model is also well-suited to weakly compressible flows, as it is able to recover the correct scaling of the pressure oscillations in the limit of the Mach number M going to 0. This work aims to close a gap in the family of the BN-type model, as the proposed one is the first pressure-based two-phase model with these features.

The pressure-based BN-type model is derived from the symmetric variant with pressure and velocity relaxation proposed by Saurel and Abgrall [1]. To allow for generic equations of state, the speed of sound for each phase i is defined as

$$c_i^2 = \chi_i + \kappa_i \frac{P_i + e_i}{\rho_i}, \qquad \text{where} \quad \chi = \left(\frac{\partial P}{\partial \rho}\right)_e \quad \text{and} \quad \kappa = \left(\frac{\partial P}{\partial e}\right)_\rho. \tag{1}$$

After deriving the pressure formulation, we apply a special pressure scaling that filters out the acoustics associated to long waves. Performing a multiple space scale asymptotic analysis, the pressure can be composed by three major contributions, i.e., $P = P^{(0)} + MP^{(1)} + M^2P^{(2)} + \mathcal{O}(M^3)$, among which: the $P^{(0)}$ is the thermodynamic variable, $P^{(2)}$ is responsible for local force balance, and $P^{(1)}$ is associated to long wave acoustics, which can be neglected in the zero Mach number limit for bounded domains [2]. Hence, the dimensionless pressure is defined as deviation from a reference pressure P_r, scaled with respect to reference density ρ_r and velocity u_r, that is $P = \left(\tilde{P} - P_r\right)/\rho_r u_r^2$. This definition affects the scaling of all thermodynamic quantities. Notably, the relation between the dimensionless speed of sound c and its dimensional counterpart $\tilde{c}$ (omitting the

subscript i of the phase for brevity) is $\tilde{c}^2 = \left[c^2 + \frac{\kappa}{M_r^2 \rho}\right] u_r^2$ where $M_r^2 = \frac{\rho_r u_r^2}{P_r}$ is the reference Mach number, which should be expression of the global level of compressibility of the flow field.

The resulting dimensionless pressure-based BN-type model reads [3]

$$\frac{\partial \alpha_i}{\partial t} = -u_{\mathrm{IN}} \frac{\partial \alpha_i}{\partial x} - \mu \Delta_i P \tag{2}$$

$$\frac{\partial (\alpha_i \rho_i)}{\partial t} + \frac{\partial (\alpha_i \rho_i u_i)}{\partial x} = 0 \tag{3}$$

$$\frac{\partial (\alpha_i \rho_i u_i)}{\partial t} + \frac{\partial (\alpha_i \rho_i u_i^2 + \alpha_i P_i)}{\partial x} = P_{\mathrm{IN}} \frac{\partial \alpha_i}{\partial x} + \lambda \Delta_i u \tag{4}$$

$$\begin{aligned} M_r^2 \left[\alpha_i \frac{\partial P_i}{\partial t} + \alpha_i u_i \frac{\partial P_i}{\partial x} + (\alpha_i \rho_i c_i^2) \frac{\partial u_i}{\partial x} \right] &= \kappa_i \left[u_{\mathrm{IN}} \frac{\partial \alpha_i}{\partial x} + \mu \Delta_i P - \frac{\partial (\alpha_i u_i)}{\partial x} \right] \\ + M_r^2 \left[\rho_i c_{i,\mathrm{IN}}^2 (u_{\mathrm{IN}} - u_i) \left(\frac{\partial \alpha_i}{\partial x} + \mu P_{\mathrm{IN}} \Delta_i P \right) + \kappa_i \lambda (u_{\mathrm{IN}} - u_i) \Delta_i u \right] \end{aligned} \tag{5}$$

where P_{IN} and u_{IN} are the interface pressure and velocity, defined as weighted averages between the phases, and $c_{i,\mathrm{IN}}$ is the interface speed of sound, a variable without thermodynamic meaning, but defined as the speed of sound c_i in (1), considering P_{IN} instead of P_i. The operator Δ_i indicates the jump in the variable phase i and the other, with opposite sign, and λ and μ are relaxation parameters.

The model (2)–(5) recovers the correct scaling in the zero-Mach limit thanks to the peculiar shape of Eq. (5), which, for $M_r \to 0$, reduces to $\frac{\partial \alpha_i}{\partial t} + \frac{\partial \alpha_i u_i}{\partial x} = 0$, which expresses the multi-phase counterpart of the divergence-free condition for single-phase incompressible flows.

To solve the governing equations (2)–(5), a splitting approach is adopted, so the solution at the time t^{n+1} is obtained in two steps: first, the hyperbolic part of the PDEs including the temporal, the convective and the non-conservative terms is solved; then, the ODEs associated to the relaxation terms are integrated.

Standard numerical techniques are combined to build the hyperbolic operator, which applies a segregate solution strategy, as it is common in pressure-based solvers. Hence, after solving the volume fraction and mass equation for each phase, the momenta for each phase are predicted evaluating the pressure gradient at the time t^n. Then, the pressure equations are solved and the momenta are updated. A semi-implicit time integration is used to avoid an excessively stringent stability condition on the time step due to the low Mach, treating implicitly the acoustic terms. To integrated implicitly the divergence of the velocity in the pressure equation, an approximation for the velocities u_i^{n+1} is derived by the momentum update equations. As a consequence of this choice, due to the chosen definition of P_{IN}, the pressure equations of the two phases are coupled [3].

A finite volume scheme over a staggered grid is used to spatially discretized the governing equations. The non-conservative terms, involving the gradient of the volume fraction, are discretized following the non-disturbance condition, stating that a two-phase flow uniform in pressure and velocity at t^n must remain uniform

in these variables at time t^{n+1} [4]. This procedure leads to a discetization that depends on the fluxes used for the convective terms, here the Rusanov fluxes, but it is robust.

Finally, the relaxation operator uses a backward Euler scheme to integrate

$$\frac{\mathrm{d}\alpha_1}{\mathrm{d}t} = \mu\Delta_1 P\,; \qquad \frac{\mathrm{d}\alpha m_i}{\mathrm{d}t} = -\lambda\Delta_i u\,, \quad \text{for } i = \{1,2\}$$
$$M_r^2\alpha_i\frac{\mathrm{d}P_i}{\mathrm{d}t} = -\left[M_r^2\rho_i c_{i,\mathrm{IN}}^2 + \kappa_i\right]\mu\Delta_i P - M_r^2\kappa_i(u_{\mathrm{IN}} - u_i)\lambda\Delta_i u\,, \quad \text{for } i = \{1,2\}\,.$$

The momentum equations are solved straightforwardly, whereas the system involving the volume fraction and the pressure equations requires some care, as it is highly non-linear, especially when using complex equations of state, and stiff.

The validity of the developed simulation tool is shown through one-dimensional shock-tube tests, involving water-aluminum and almost pure flows. The numerical results show a good agreement with reference ones, even at acoustic CFL numbers greater than one, but some expected discrepancies across shocks, where however the errors remain acceptable (within some percentage points). The effects of different values of relaxation parameters are investigated: large values lead to results similar to the one predicted by assuming mechanical equilibrium between the phase, whereas a decrease of relaxation parameters (especially λ) leads to a smoothing of the expansion and compression waves. Finally, a shock-tube containing a two-phase CO_2 mixture at saturation conditions is simulated, modeling the fluids with the Peng–Robinson equation of state. The results illustrate how the proposed full non-equilibrium BN-type model allows each phase to evolve independently according to its own thermodynamic model, although the equilibrium is enforced at the interfaces: the state of each phase evolves in close proximity to the saturation curve, but only the evolution of the mixture density develops in the fully two-phase region.

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Godunov-Type Numerical Fluxes for Diffusion

Claus-Dieter Munz
(joint work with Steven Jöns, Johanna Hintz, Christoph Müller)

For finite volume or discontinuous Galerkin schemes, the use of the Riemann problem solution to construct the numerical fluxes is a standard approach that started with the work of Godunov. Gassner et al. initiated in [1] the use of the Riemann problem solution to construct diffusive fluxes later. This is an alternative to the more common approach to reconstruct the gradients for the diffusive fluxes by assuming continuity across the grid cell interfaces. The latter approach is motivated by the regularizing property of the parabolic terms. If a phase interface is approximated as a discontinuity within the macroscopic description the continuity assumption is at least questionable. Here, the generalized diffusive Riemann problem, which allows to determine directly heat and viscous flux from the discontinuous data seems to be more appropriate.

The procedure for the scalar case can be extended to the thermal and viscous fluxes of the Navier Stokes into normal direction. Hence, we first consider the one-dimensional diffusion equation with discontinuous coefficients for the scalar diffusion equation

$$u_t - (\lambda u_\xi)_\xi = 0 \tag{1}$$

with piecewise linear initial data

$$u(\xi, t=0) = \begin{cases} u^- + \xi u_\xi^- & \text{for} \quad \xi < 0 \\ u^+ + \xi u_\xi^+ & \text{for} \quad \xi \geq 0 \end{cases} \tag{2}$$

and with the positive piecewise constant diffusion coefficient

$$\lambda(\xi) = \begin{cases} \lambda^- & \text{for} \quad \xi < 0, \\ \lambda^+ & \text{for} \quad \xi \geq 0. \end{cases} \tag{3}$$

The nomination is such that "-" and "+" denote the values and functions on the left hand and on the right hand side, respectively. Our considerations here are based on the work of Lörcher et al. [1] with a generalization of the compatibility condition.

By Laplace transformation one obtains a left second order ordinary differential equation and a right one. The general solution of both sides can be calculated and every solution has two integration constants. One constant at every side is set to Zero to get the bounded part of the solutions only. The other two constants are determined by compatibiliy conditions at $\xi = 0$, which state that the solution and the diffusion flux is continuous.

The dervivatives of the solution at $\xi = 0$ read as

$$\partial_\xi u^-(0,t) = \frac{u^+ - u^-}{\sqrt{\pi t}(\sqrt{\lambda^-} + \sqrt{\lambda^+})} + \frac{\sqrt{\lambda^+}u_\xi^+ + \sqrt{\lambda^-}u_\xi^-}{\sqrt{\lambda-} + \sqrt{\lambda^+}}, \tag{4a}$$

$$\partial_\xi u^+(0,t) = \frac{u^+ - u^-}{\sqrt{\pi t}(\sqrt{\lambda^-} + \sqrt{\lambda^+})} + \frac{\sqrt{\lambda^+}u_\xi^+ + \sqrt{\lambda^-}u_\xi^-}{\sqrt{\lambda^+} + \sqrt{\lambda^+}}. \tag{4b}$$

The diffusion fluxes are then obtained by taking the integral mean over one time step. We note that the derivatives are singular at $\xi = 0$ as derivatives of a discontinuous function. However, the time average exists as an improper integral and reads as

$$g(u^-, u^+, u_\xi^-, u_\xi^+) = \frac{2\sqrt{\lambda^+\lambda^-}(u^+ - u^-)}{\sqrt{\pi\Delta t}(\sqrt{\lambda^-} + \sqrt{\lambda^+})} + \frac{\sqrt{\lambda^+}u_\xi^+ + \sqrt{\lambda^-}u_\xi^-}{\sqrt{\lambda^-} + \sqrt{\lambda^+}}. \tag{5}$$

The time step Δt has to satisfy the parabolic stability condition.

This solution is used to define a heat flux for the Navier Stokes equations. It turned out that it is better to impose the continuity of the heat flux from the energy equation before its reformulation into a temperature equation. The extension to the viscous terms is more subtle. The viscosity matrix is evaluated at the weighted

$$\bar{u} = \frac{\sqrt{\lambda^+}u^+ + \sqrt{\lambda^-}u^-}{\sqrt{\lambda^+} + \sqrt{\lambda^-}}. \tag{6}$$

Then the viscosity matrix can be diagonalized and the scalar approach is applied to each characteristic field, see [2].

Riemann problems for the Navier Stokes equations which contain an material interface with a temperature jump and a jump in the viscous terms indicate that this approach works very well. This method is also applied to the two-phase simulutions using the ghost flux mathod to keep the interface sharp that has been developed in [3].

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On the preservation of curl involutions in Newtonian continuum mechanics and general relativistic continuum phyiscs

Michael Dumbser

(joint work with Saray Busto, Simone Chiocchetti, Francesco Fambri, Elena Gaburro, Sergey Gavrilyuk, Ilya Peshkov, Anne Reinarz)

In this report we discuss an extension of the generalized Lagrangian multiplier method (GLM) of Munz et al. [9, 4], which was originally conceived for the numerical solution of the Maxwell and MHD equations with divergence-type involutions, to the case of hyperbolic PDE systems with curl-type involutions. The key idea here is to solve an *augmented* PDE system, in which curl errors are propagated away via an additional Maxwell-type subsystem that is coupled to the PDE containing the involution at the aid of an additional cleaning vector. The new approach is presented on a simple model problem, in order to explain the basic ideas. We discuss the cleaning of homogeneous and non-homogeneous curl involutions. Our new GLM curl cleaning method was already successfully applied to a first order hyperbolic model for surface tension [13, 3] and to a first order hyperbolic reformulation of the nonlinear Schrödinger equation of quantum hydrodynamics [5, 2]. The GLM cleaning proposed by Busto *et al.* in [2] is the first one to be also *thermodynamically compatible* with the total energy conservation law (thermodynamically compatible GLM curl cleaning) in the sense that the total energy conservation equation can be obtained as a linear combination of all the other equations, including the cleaning vector, following the framework of Godunov and Romenski of symmetric hyperbolic and thermodynamically compatible (SHTC) systems, see e.g. [7, 12]. Finally, applications to a strongly hyperbolic first order reduction of the CCZ4 formulation (FO-CCZ4) of the Einstein field equations of general relativity, which is endowed with 11 curl constraints, can be found in [6]. The main advantages of the proposed GLM approach are its complete independence of the underlying numerical scheme and grid topology and its easy implementation into existing numerical methods and computer codes. Furthermore, in Newtonian continuum models we were able to show that the method allows to restore strong hyperbolicity of originally weakly hyperbolic systems. It is furthermore compatible with the conservation of total energy and momentum, unlike the classical Godunov-Powell terms [8, 11]. However, this flexibility comes at the price of needing to add for each curl involution one additional 3 vector plus another scalar in the augmented system for homogeneous curl constraints, and even two additional 3 vectors and 2 scalars for non-homogeneous curl involutions.

Here we briefly recall the original hyperbolic GLM divergence cleaning approach of Munz et al. [9, 4] for the Maxwell and MHD equations. Throughout this paper we employ the Einstein summation convention, which implies summation over two repeated indices. Furthermore, we will use Latin indices ranging from 1 to 3. We furthermore use the notation $\partial_t = \partial/\partial t$, $\partial_k = \partial/\partial x_k$ and ε_{ijk} is the usual fully anti-symmetric Levi-Civita symbol. The induction equation in electrodynamics

reads

$$\partial_t B_k + \varepsilon_{kij} \partial_i E_j = 0, \tag{1}$$

with the magnetic field B_k and the electric field E_j. A consequence of the above induction equation is the famous divergence-free condition

$$\mathcal{I} = \partial_m B_m = 0 \tag{2}$$

of the magnetic field, which states that there exist no magnetic monopoles, or, in other words, the magnetic field will remain divergence-free for all times if it was initially divergence-free.

One way to preserve a divergence-free magnetic field within a numerical scheme is the use of an exactly divergence-free discretization on appropriately staggered meshes, see e.g. [14, 1]. However, the implementation of such exactly structure-preserving methods into an existing code is rather invasive and often requires substantial changes in the algorithm structure of existing general purpose solvers for hyperbolic conservation laws that were not right from the beginning designed for the solution hyperbolic PDE with involution constraints. The very popular GLM method proposed by Munz et al. in [9, 4] is an alternative to exactly constraint–preserving schemes and requires only a rather small change *at the PDE level*, where simply an additional equation for a cleaning scalar ϕ is added to the system, so that divergence errors cannot accumulate locally any more, but instead are transported away under the form of acoustic-like waves with finite speed. This approach is very easy to implement in any general purpose CFD code and is completely independent of the underlying numerical scheme or mesh topology. The role of the cleaning scalar ϕ is the one of a generalized Lagrangian multiplier (GLM) that accounts for the involution constraint. The way how it works can best be explained with a physical example, which is the role of the pressure in the compressible Euler equations: for low Mach numbers (i.e. for large sound speed compared to the flow speed), the coupling of the momentum equation with the pressure equation drives the divergence of the velocity field to zero for $M \to 0$. In the same manner, the evolution equation of the additional cleaning scalar ϕ coupled with the induction equation drives the divergence of the magnetic field to zero if the cleaning speed is chosen large enough. The *augmented induction equation* according to the GLM approach of Munz et al. [9, 4] therefore reads

$$\partial_t B_k + \varepsilon_{kij} \partial_i E_j + \partial_k \varphi = 0, \tag{3}$$

$$\partial_t \varphi + a_d^2 \, \partial_m B_m = 0, \tag{4}$$

with the new cleaning scalar φ, an *artificial* cleaning speed a_d. The new terms in the augmented system (3) and (4) with respect to the original equation (1) are highlighted in red, for convenience. It is easy to see that for $a_d \to \infty$ the equation (4) leads to $\partial_m B_m \to 0$, which is the above involution (2).

We show the basic idea of our new GLM curl cleaning approach on a simple toy model, in order to ease notation and to facilitate the understanding of the underlying concepts. For details and successful applications to complex systems,

the reader is referred to [6, 3, 2]. Consider the following evolution system for one scalar ρ and two vector fields v_k and J_k,

$$\partial_t \rho + \partial_i \left(\rho v_i\right) = 0, \tag{5}$$

$$\partial_t (\rho v_k) + \partial_i \left(\rho v_i v_k + \rho c_0^2 J_i J_k\right) = 0, \tag{6}$$

$$\partial_t J_k + \partial_k (v_m J_m) + v_m \left(\partial_m J_k - \partial_k J_m\right) = 0, \tag{7}$$

with c_0 a given constant. Defining a scalar quantity $\chi = v_m J_m$ and with the use of the Schwarz theorem $\partial_k \partial_m \chi = \partial_m \partial_k \chi$ (symmetry of second derivatives) it is very easy to see that the second PDE above, eqn. (7), is endowed with the linear involution constraint

$$\mathcal{I}_{mk} = \partial_m J_k - \partial_k J_m = 0. \tag{8}$$

This means that if $\mathcal{I}_{mk} = 0$ at the initial time, it will remain zero for all times. Indeed, one can immediately notice that the term $\partial_k (v_m J_m)$ is the gradient of a scalar, the curl of which is zero, and that the involution itself is contained in the third term on the left hand side of eqn. (7), which is needed to make the system Galilean invariant.

As already mentioned before, the main advantage of the GLM approach of Munz et al. [9, 4] for divergence constraints is not only the ease of implementation, but also its great *flexibility* and its compatibility with *all* types of mesh topologies and numerical schemes, since it only requires the solution of an additional scalar PDE for the cleaning scalar, which can easily be added to an existing code.

The extended GLM curl cleaning proposed in this paper can now be explained on the toy system (6)-(7) as follows. The original governing PDE system (6) and (7) is simply *replaced* by the following *augmented system*

$$\partial_t \rho + \partial_i \left(\rho v_i\right) = 0, \tag{9}$$

$$\partial_t (\rho v_k) + \partial_i \left(\rho v_i v_k + \rho c_0^2 J_i J_k\right) = 0, \tag{10}$$

$$\partial_t J_k + \partial_k (v_m J_m) + v_m \left(\partial_m J_k - \partial_k J_m\right) + \varepsilon_{klm} \partial_l \psi_m = 0, \tag{11}$$

$$\partial_t \psi_k - a_c^2 \, \varepsilon_{klm} \partial_l J_m + \partial_k \varphi = 0 \tag{12}$$

$$\partial_t \varphi + a_d^2 \, \partial_m \psi_m = 0, \tag{13}$$

where a_c is a new cleaning speed associated with the curl cleaning. The new terms associated with the curl cleaning are highlighted in blue. Since the evolution equation for the cleaning field ψ_k has formally the same structure as the induction equation (1) of the Maxwell equations, it is again endowed with the divergence-free constraint $\partial_m \psi_m = 0$, which is taken into account via the classical GLM method (red terms). It is easy to see that from (12) for $a_c \to \infty$ we obtain $\epsilon_{klm} \partial_l J_m \to 0$ in the limit, thus satisfying the involution in the sense $\mathcal{I}_{mk} \to 0$. The augmented system (9)-(13) can now be solved with any standard numerical method for nonlinear systems of hyperbolic partial differential equations.

In case the curl involutions are *not* homogeneous, but where the curl has to assume a prescribed non-zero value, which is the case when the evolution equation

(7) for J_k contains a nonlinear source term S_k whose curl does not vanish,

$$\partial_t J_k + \partial_k(v_m J_m) + v_m \left(\partial_m J_k - \partial_k J_m\right) = S_k, \tag{14}$$

see [10], then the following strategy can be used: We first define the curl of $\mathbf{J}$ to be equal to another quantity

$$B_i = \varepsilon_{ijk}\partial_j J_k, \tag{15}$$

which according to [10] is the so-called *Burgers vector*. Its evolution equation can be obtained by taking the curl of (14), leading to the following additional evolution equation (see Appendix C of [10]):

$$\partial_t B_i + \partial_k \left(B_i v_k - v_i B_k - \varepsilon_{ikj} S_j\right) + v_i\, \partial_k B_k = 0. \tag{16}$$

Directly from its definition (15) it is obvious that the Burgers vector must be divergence-free, i.e. $\partial_k B_k = 0$. The divergence constraint on the Burgers vector is explicitly contained in (16) in order to achieve a Galilean invariant formulation. Therefore, the GLM approach for a general, non-trivial curl of J_k reads as follows:

$$\partial_t \rho + \partial_i \left(\rho v_i\right) = 0, \tag{17}$$

$$\partial_t(\rho v_k) + \partial_i \left(\rho v_i v_k + \rho c_0^2 J_i J_k\right) = 0, \tag{18}$$

$$\partial_t J_k + \partial_k(v_m J_m) + v_m \left(\partial_m J_k - \partial_k J_m\right) + \varepsilon_{klm}\partial_l \psi_m = S_k, \tag{19}$$

$$\partial_t B_i + \partial_k \left(B_i v_k - v_i B_k - \varepsilon_{ikj} S_j\right) + v_i \partial_k B_k + \partial_i \chi = 0, \tag{20}$$

$$\partial_t \psi_k - a_c^2\, \varepsilon_{klm}\partial_l J_m + \partial_k \varphi = -a_c^2 B_k \tag{21}$$

$$\partial_t \varphi + a_d^2\, \partial_m \psi_m = 0, \tag{22}$$

$$\partial_t \chi + a_b^2\, \partial_m B_m = 0. \tag{23}$$

Here, we have used the usual blue color for the curl cleaning, the red color for the divergence cleaning and the green color due to the additional terms and equations that are necessary in the case the curl of $\mathbf{J}$ is equal to a non-zero Burgers vector. It is again obvious that for $a_c \to \infty$ we obtain $\varepsilon_{ijk}\partial_j J_k \to B_i$, i.e. the involution (15).

We illustrate the effectiveness of the proposed GLM cleaning approach on a numerical example taken from [3], i.e. the dynamics of an oscillating bubble. The governing equations are endowed with a curl involution and without GLM cleaning or Godunov-Powell terms the system is only weakly hyperbolic. From Figure 1 it can be clearly seen that the original weakly hyperbolic system is unstable after short time, the Godunov-Powell terms, which restore strong hyperbolicity, but which are not conservative for total energy and momentum are able to stabilize the simulation, while the best results are obtained with the new hyperbolic GLM curl cleaning, which does not only restore strong hyperbolicity, but which also conserves momentum and total energy.

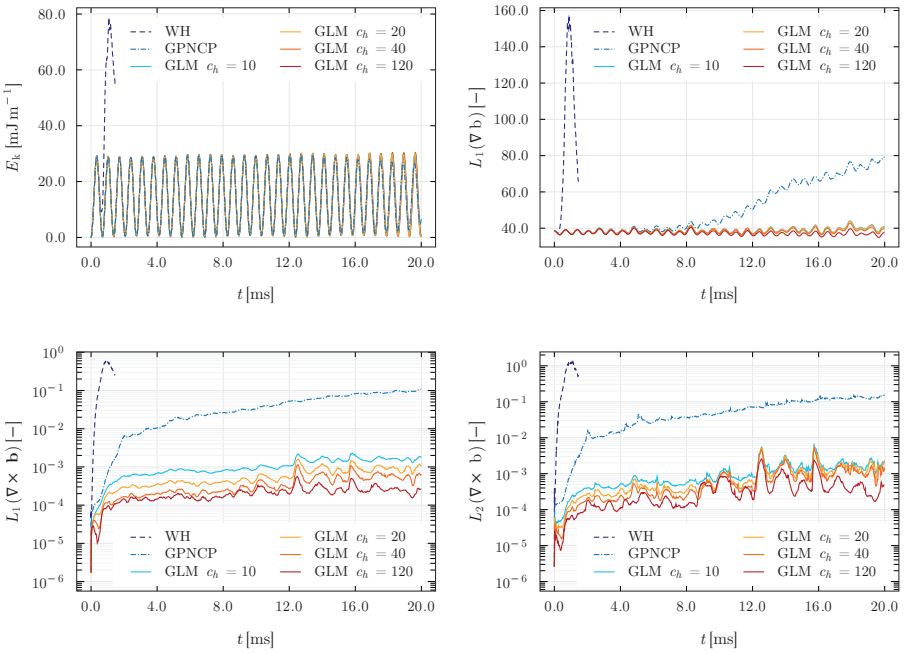

FIGURE 1. Time evolution of global dynamics and of curl errors for an oscillating bubble. Top row, left to right: total kinetic energy and L_1 norm of the gradient field $\nabla \mathbf{b}$ over time. Bottom row: the timeseries for the L_1 and L_2 norms of the curl error. The simulations employed a sixth order ADER-DG scheme with third order ADER-WENO subcell finite volume limiter uniform Cartesian grid composed of 64^2 elements.

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The role of curl-type involutions in continuum physics

Ilya Peshkov

In the nonlinear elasticity theory, the curl $\partial_i A^A_{\ k} - \partial_k A^A_{\ i}$ of the distortion field $A^A_{\ k} = \frac{\partial \xi^A}{\partial x^k}$, $A = 1,2,3$, $i,k = 1,2,3$ 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 and the time evolution of the distortion field are, in fact, projection of a space-time identity

$$\partial_\mu A^a_{\ \nu} - \partial_\nu A^a_{\ \mu} = 0, \tag{1}$$

$a = 0,1,2,3$, $\mu,\nu = 0,1,2,3$, with ∂_0 being the time derivative.

We shall discuss that, if generalized to

$$\partial_\mu A^a_{\ \nu} - \partial_\nu A^a_{\ \mu} = T^a_{\ \mu\nu}, \tag{2}$$

i.e. we admit that the 4-curl of the four-distortion $A^a_{\ \mu}$ is not zero, this type of time evolution equations is fundamentals for such a physical theory as the Yang-Mills gauge theory and mathematical theory as the Riemann-Cartan geometry.

From the perspective of modeling in continuum mechanics, (2) was fundamental for building the unified inelasticity theory [1] which is able to describe in a unified manner elastic/inelastic solids and viscous fluids in a single system of PDEs. Moreover, we shall discuss how the evolution equations of the type (2) can be used for modeling turbulence flows and modeling dispersive phenomena such as a frequency band-gap in acoustic metamaterials [2].

Finally, we also pay certain attention to a discussion of the importance of developing structure preserving numerical methods in order to properly discretize the curl-type evolution equation of the form (2).

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Generalized Rankine – Hugoniot relations for multi-dimensional shocks in dispersive media

Sergey Gavrilyuk

The Euler equations of compressible fluids, hyperelasticity, MHD, etc. are typical examples of hyperbolic systems of conservation laws admitting shock solutions, i.e. discontinuous solutions satisfying the governing equations in a weak sense. The corresponding equations of motion are the Euler-Lagrange equations for a functional which is the Hamilton action. The dispersive regularizations of these models based on the modification of the corresponding Lagrangian aim at avoiding discontinuities by replacing them by "dispersive shocks", i.e. by strongly oscillating non stationary fronts.

We show that in some cases dispersive regularization produces solutions that are "almost" classical shocks. Such solutions must necessarily satisfy special jump relations (generalized Rankine-Hugoniot relations) that follow naturally from the variational structure of the governing equations.

I will consider the Benjamin-Bona-Mahony (BBM) equation as a toy model to study these unusual shock solutions. The BBM equation is a simplest unidirectional model of shallow water waves. As we will see, it has stable discontinuous solutions.

I will also explain how the generalised jump relations for dispersive equations can be used to explain, in particular, the Leidenfrost phenomenon (or the film boiling phenomenon) which was the main reason for the nuclear accidents in Chernobyl (1986) and in Fukushima (2011).

This is a joint work with H. Gouin (AMU, Marseille) and K. M. Shyue (NTU, Taiwan) [1, 2, 3]

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Thermodynamically compatible finite volume schemes for continuum mechanics

Saray Busto
(joint work with Michael Dumbser, Ilya Peshkov, Evgeniy Romenski)

The Godunov-Peskov-Romenski (GPR) model is a first order symmetric hyperbolic and thermodynamically compatible (SHTC) PDE system that is able to describe continuum mechanics from nonlinear elastoplastic solids at large deformations to viscous fluids. This is achieved at the aid of suitable relaxation source terms, making it a powerful tool to model numerous physical phenomena. One of the main challenges concerning the development of numerical methods for this kind of systems consists in preserving the thermodynamic compatibility of the equations also at the discrete level. To this end, we propose constructing a discrete framework for the compressible Euler equations mimicking the continuous formalism introduced by Godunov in 1961, see [1]. The remaining terms in the more general GPR model, including non-conservative products, are 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, the HTC scheme proposed is provably marginally stable in the energy norm and satisfies a discrete entropy inequality by construction, see [2]. We stress that a key feature of our new scheme is that it directly discretizes the *entropy inequality* and obtains the energy conservation law as a *consequence* of the thermodynamically compatible discretization of all the other equations.

1. Mathematical model

We consider the first order hyperbolic model of continuum mechanics, regularized with vanishing viscosity terms which goes back to the work of Godunov, Peshkov & Romenski [1, 3, 4, 5, 6, 7]:

$$
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_k)}{\partial x_k} - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial \rho}{\partial x_m}\right) = 0,\\
&\frac{\partial \rho v_i}{\partial t} + \frac{\partial\left(\rho v_i v_k + p\,\delta_{ik} + \sigma_{ik} + \omega_{ik}\right)}{\partial x_k} - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial \rho v_i}{\partial x_m}\right) = 0,\\
&\frac{\partial \rho S}{\partial t} + \frac{\partial\left(\rho S v_k + \beta_k\right)}{\partial x_k} - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial \rho S}{\partial x_m}\right) = \Pi + \frac{\alpha_{ik}\alpha_{ik}}{\theta_1(\tau_1)T} + \frac{\beta_i \beta_i}{\theta_2(\tau_2)T} \geq 0,\\
&\frac{\partial A_{ik}}{\partial t} + \frac{\partial(A_{im} v_m)}{\partial x_k} + v_m\left(\frac{\partial A_{ik}}{\partial x_m} - \frac{\partial A_{im}}{\partial x_k}\right) - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial A_{ik}}{\partial x_m}\right) = -\frac{\alpha_{ik}}{\theta_1(\tau_1)},\\
&\frac{\partial J_k}{\partial t} + \frac{\partial\left(J_m v_m + T\right)}{\partial x_k} + v_m\left(\frac{\partial J_k}{\partial x_m} - \frac{\partial J_m}{\partial x_k}\right) - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial J_k}{\partial x_m}\right) = -\frac{\beta_k}{\theta_2(\tau_2)},\\
&\frac{\partial \mathcal{E}}{\partial t} + \frac{\partial\left(v_k\left(\mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 + \mathcal{E}_4\right) + v_i\left(p\,\delta_{ik} + \sigma_{ik} + \omega_{ik}\right) + h_k\right)}{\partial x_k} - \frac{\partial}{\partial x_m}\left(\epsilon \frac{\partial \mathcal{E}}{\partial x_m}\right) = 0,
\end{aligned}
$$

where $\mathbf{q} = \{q_i\} = (\rho, \rho v_i, \rho S, A_{ik}, J_k)^T$ denotes the state vector, $\mathcal{E} = \rho E = \mathcal{E}_1 + \mathcal{E}_2 + \mathcal{E}_3 + \mathcal{E}_4$ is the total energy potential, $\mathcal{E}_i = \rho E_i$, $\epsilon > 0$ is a vanishing viscosity and the nonnegative entropy production term due to the viscous terms is given by

$$\Pi = \frac{\epsilon}{T}\, \partial_{x_m} q_i \; \partial^2_{q_i q_j} \mathcal{E}\, \partial_{x_m} q_j \geq 0.$$

In the above model the four contributions to the total energy density are

$$\mathcal{E}_1 = \frac{\rho^\gamma}{\gamma - 1} e^{S/c_v}, \quad \mathcal{E}_2 = \frac{1}{2}\rho v_i v_i, \quad \mathcal{E}_3 = \frac{1}{4}\rho c_s^2 \mathring{G}_{ij}\mathring{G}_{ij}, \quad \mathcal{E}_4 = \frac{1}{2} c_h^2 \rho J_i J_i,$$

with $\mathbf{G} = A_{ji}A_{jk}$ the metric tensor and $\mathring{\mathbf{G}}$ its trace-free part. The vector of thermodynamic dual variables reads $\mathbf{p} = \partial_{\mathbf{q}}\mathcal{E} = \{p_i\} = (r, v_i, T, \alpha_{ik}, \beta_k)^T$ with

$$r = \partial_\rho \mathcal{E}, \qquad v_i = \partial_{\rho v_i}\mathcal{E}, \qquad T = \partial_{\rho S}\mathcal{E}, \qquad \alpha_{ik} = \partial_{A_{ik}}\mathcal{E}, \qquad \beta_k = \partial_{J_k}\mathcal{E}.$$

The pressure is defined as $p = \rho\, \partial_\rho \mathcal{E} + \rho v_i\, \partial_{\rho v_i}\mathcal{E} + \rho S\, \partial_{\rho S}\mathcal{E} - \mathcal{E} = \rho^2 \partial_\rho E$, the stress tensors due to shear stress and thermal stress are, respectively, $\sigma_{ik} = A_{ji}\alpha_{jk}$, $\omega_{ik} = J_i \beta_k$, while the heat flux vector is given by $h_k = T\beta_k$. Furthermore, $\theta_1(\tau_1) > 0$ and $\theta_2(\tau_2) > 0$ are two algebraic functions of the state vector $\mathbf{q}$ and the positive relaxation times $\tau_1 > 0$ and $\tau_2 > 0$:

$$\theta_1 = \frac{1}{3}\rho z_1 \tau_1\, c_s^2\, |\mathbf{A}|^{-\frac{5}{3}}, \qquad \theta_2 = \rho z_2 \tau_2\, c_h^2, \qquad z_1 = \frac{\rho_0}{\rho}, \qquad z_2 = \frac{\rho_0 T_0}{\rho T}$$

with ρ_0 and T_0 being some reference density and temperature.

In [7] a formal asymptotic analysis of the model (1)-(1) was carried out, revealing that in the stiff limit the stress tensor σ_{ik} and the heat flux h_k tend to

$$\sigma_{ik} = -\frac{1}{6}\rho_0 c_s^2 \tau_1 \left(\partial_k v_i + \partial_i v_k - \frac{2}{3}\left(\partial_m v_m\right)\delta_{ik} \right), \qquad h_k = -\rho_0 T_0 c_h^2 \tau_2 \partial_k T,$$

i.e. when the relaxation times $\tau_1, \tau_2 \to 0$, the Navier-Stokes-Fourier equations are retrieved with effective shear viscosity $\mu = \frac{1}{6}\rho_0 c_s^2 \tau_1$ and heat conductivity $\kappa = \rho_0 T_0 c_h^2 \tau_2$.

Computing the dot product of the thermodynamic dual variables with the system of equations but the energy, we obtain the energy equation as a direct consequence. Therefore, our objective is to develop a numerical scheme able to preserve this property also at the discrete level.

2. Thermodynamically compatible semi-discrete FV scheme in 2D

We propose the following semi-discrete finite volume scheme:

$$\frac{\partial \rho^\ell}{\partial t} = -\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| D_\rho^{\ell r,-} + \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| g_{\rho,\,\mathbf{n}}^{\ell r},$$

$$\frac{\partial (\rho v_i^\ell)}{\partial t} = -\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| D_{\rho v_i}^{\ell r,-} - \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \sigma_{ik}^{\ell r,-} n_k$$
$$-\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \omega_{ik}^{\ell r,-} n_k + \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| g_{\rho v_i,\,\mathbf{n}}^{\ell r},$$

$$\frac{\partial (\rho S^\ell)}{\partial t} = -\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| D_{\rho S}^{\ell r,-} - \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \left(\beta_k^{\ell r} - \beta_k^\ell\right) n_k$$
$$+\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| g_{\rho S,\,\mathbf{n}}^{\ell r} + \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \Pi_{\mathbf{n}}^{\ell r,-} + \frac{\alpha_{ik}^\ell \alpha_{ik}^\ell}{\theta_1^\ell(\tau_1)\,T^\ell} + \frac{\beta_i^\ell \beta_i^\ell}{\theta_2^\ell(\tau_2)\,T^\ell},$$

$$\frac{\partial A_{ik}^\ell}{\partial t} = -\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \frac{1}{2} A_{im}^{\ell r}\left(v_m^r - v_m^\ell\right) n_k - \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \frac{1}{2}\tilde{u}_{A,\,\mathbf{n}}^{\ell r}\left(A_{ik}^r - A_{ik}^\ell\right)$$
$$+\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| g_{A_{ik},\,\mathbf{n}}^{\ell r} - \frac{\alpha_{ik}^\ell}{\theta_1^\ell(\tau_1)},$$

$$\frac{\partial J_k^\ell}{\partial t} = -\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \frac{1}{2} J_i^{\ell r}\left(v_m^r - v_m^\ell\right) n_k - \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \frac{1}{2} T^{\ell r,-} n_k$$
$$-\frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| \frac{1}{2}\tilde{u}_{J,\,\mathbf{n}}^{\ell r}\left(J_k^r - J_k^\ell\right) + \frac{1}{|\Omega^\ell|}\sum_{r\in N_\ell}\left|\partial\Omega^{\ell r}\right| g_{J_k,\,\mathbf{n}}^{\ell r} - \frac{\beta_i^\ell}{\theta_2^\ell(\tau_2)}$$

with

$$D_{\mathbf{q}}^{\ell r,-} = \left(f_{\mathbf{q},\,k}^{\ell r} - f_{\mathbf{q},\,k}^\ell\right) n_k,$$

$$g_{\mathbf{q},\,\mathbf{n}}^{\ell r} = \epsilon^{\ell r}\frac{\mathbf{q}^r - \mathbf{q}^\ell}{\delta^{\ell r}} = \epsilon^{\ell r}\frac{\Delta\mathbf{q}^{\ell r}}{\delta^{\ell r}}, \quad \delta^{\ell r} = \left\|\mathbf{x}^r - \mathbf{x}^\ell\right\| = \Delta x n_1 + \Delta y n_2,$$

$$\sigma_{jk}^{\ell r,-} = \sigma_{jk}^{\ell r} - \sigma_{jk}^\ell, \quad \sigma_{jk}^{\ell r} = \frac{1}{2} A_{ij}^{\ell r}\left(\alpha_{ik}^\ell + \alpha_{ik}^r\right),$$

$$\omega_{jk}^{\ell r,-} = \omega_{jk}^{\ell r} - \omega_{jk}^\ell, \quad \omega_{jk}^{\ell r} = J_j^{\ell r}\frac{1}{2}\left(\beta_k^\ell + \beta_k^r\right),$$

$$\Pi_{\mathbf{n}}^{\ell r,-} = \frac{1}{2}\epsilon^{\ell r}\frac{\Delta\mathbf{q}^{\ell r}}{T^\ell}\cdot\partial_{\mathbf{qq}}^2\mathcal{E}^{\ell r}\frac{\Delta\mathbf{q}^{\ell r}}{\delta^{\ell r}}, \qquad T^\ell = \frac{\left(\rho^\ell\right)^{\gamma-1}}{(\gamma-1)\,c_v} e^{\frac{S^\ell}{c_v}},$$

$$A_{im}^{\ell r} = \frac{1}{2}\left(A_{im}^\ell + A_{im}^r\right), \qquad \tilde{u}_{A,\,\mathbf{n}}^{\ell r} = \tilde{v}_{A,\,j}^{\ell r} n_j = \frac{f_{\rho,\,j}^{\ell r} n_j\left(E_3^r - E_3^\ell\right)}{\frac{1}{2}\left(\alpha_{ik}^\ell + \alpha_{ik}^r\right)\left(A_{ik}^r - A_{ik}^\ell\right)},$$

$$J_i^{\ell r} = \frac{1}{2}\left(J_i^\ell + J_i^r\right), \quad \tilde{u}_{J,\,\mathbf{n}}^{\ell r} = \tilde{v}_{J,\,j}^{\ell r} n_j = \frac{f_{\rho,\,j}^{\ell r} n_j\left(E_4^r - E_4^\ell\right)}{\frac{1}{2}\left(\beta_k^\ell + \beta_k^r\right)\left(J_k^r - J_k^\ell\right)}, \quad T^{\ell r,-} = T^r - T^\ell.$$

This scheme admits a semi-discrete energy conservation law of the form

$$\frac{\partial \mathcal{E}^{\ell}}{\partial t} = -\frac{1}{|\Omega^{\ell}|}\sum_{r\in N_{\ell}} \left|\partial\Omega^{\ell r}\right| D_{\mathcal{E}}^{\ell r,-} + \frac{1}{|\Omega^{\ell}|}\sum_{r\in N_{\ell}} \left|\partial\Omega^{\ell r}\right| g_{\mathcal{E},\,\mathbf{n}}^{\ell r}$$

$$\text{with} \quad D_{\mathcal{E}}^{\ell r,-} + D_{\mathcal{E}}^{\ell r,+} = D_{\mathcal{E}}^{\ell r,-} + D_{\mathcal{E}}^{r\ell,-} = F^{r} - F^{\ell}.$$

Assuming that the jumps on the boundary vanish, the scheme is nonlinearly marginally stable in the energy norm, i.e. the scheme satisfies the identity

$$\int_{\Omega} \frac{\partial \mathcal{E}^{\ell}}{\partial t} dV = \sum_{\ell} |\Omega^{\ell}| \frac{\partial \mathcal{E}^{\ell}}{\partial t} = 0.$$

Moreover, assuming $T^{\ell} > 0$ and $\boldsymbol{\mathcal{H}}^{\ell r} = \partial^2_{\mathbf{qq}} \mathcal{E}^{\ell r} \geq 0$ the semi-discrete finite volume scheme satisfies the semi-discrete cell entropy inequality

$$\frac{\partial \rho S^{\ell}}{\partial t} + \sum_{r\in N_{\ell}} \frac{\left|\partial\Omega^{\ell r}\right|}{|\Omega^{\ell}|} D_{\rho S}^{\ell r,-} + \sum_{r\in N_{\ell}} \frac{\left|\partial\Omega^{\ell r}\right|}{|\Omega^{\ell}|} \left(\beta_k^{\ell r} - \beta_k^{\ell}\right) n_k - \sum_{r\in N_{\ell}} \frac{\left|\partial\Omega^{\ell r}\right|}{|\Omega^{\ell}|} g_{\rho S,\,\mathbf{n}}^{\ell r} \geq 0.$$

For further details on the derivation of the scheme and the proofs of the former results, see [2].

3. Numerical results

To analyse the behaviour of the proposed scheme in both the solid and fluid limits we employ classical benchmarks from solid mechanics and fluid dynamics, such as a solid rotor problem, a Riemann problem in a solid medium, the double shear layer and the lid driven cavity problem in a fluid, see Figure 1. In [2] detailed comparisons with available exact and numerical reference solutions have been carried out, showing the accuracy and performance of the new thermodynamically compatible finite volume scheme.

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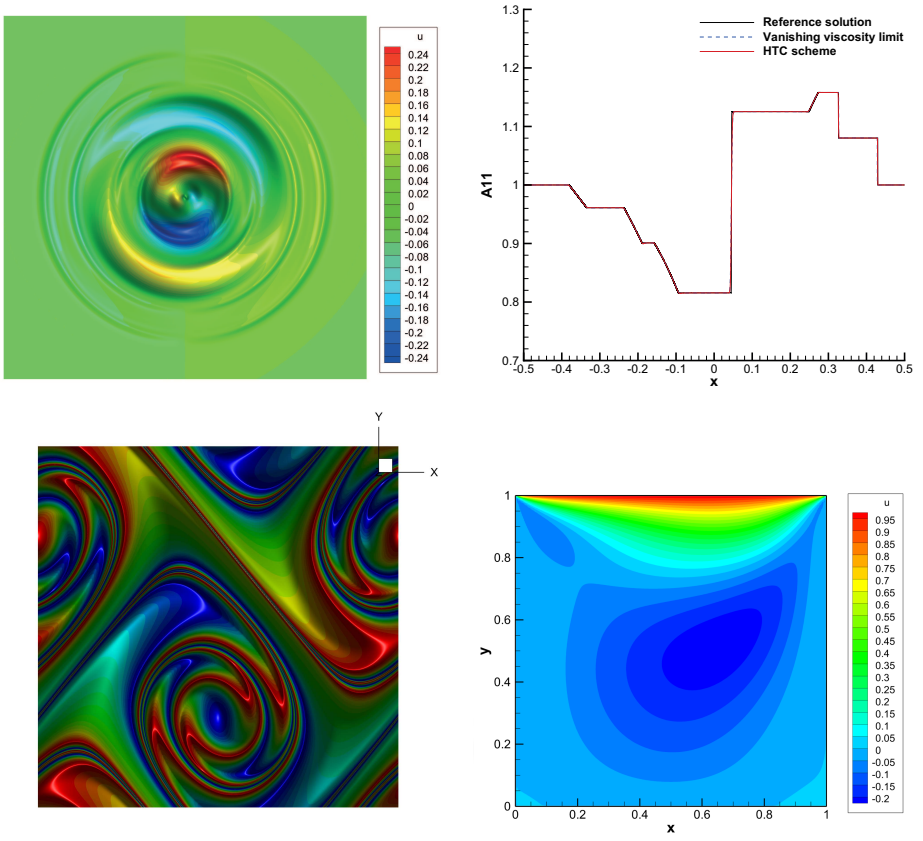

FIGURE 1. Top left: x-velocity of the solid rotor benchmark at $t = 0.3$, [8]. Top right: Riemann problem ($\rho_L = 1$, $\rho_R = 0.5$, $u_L = u_R = 0$, $v_L = -v_R = -0.2$, $p_L = 1$, $p_R = 0.5$) obtained inside a solid at $t = 0.2$ with the HTC scheme (red solid line), an ADER-DG4 scheme applied to the vanishing viscosity limit of the viscous equations, $\epsilon = 2 \cdot 10^{-5}$, (dashed blue line) and a MUSCL-Hancock scheme applied to the model with the energy conservation law (black solid line). Bottom left: Contour plot of A_{12} for the double shear layer problem, $t = 1.8$, $\mu = 2 \cdot 10^{-3}$, [9]. Bottom right: u velocity contours for the lid driven cavity problem at time $t = 10$. All results were obtained with the new HTC scheme applied to the full GPR model.

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

Mikhail Shashkov

Computational experiment is among the most significant developments in the practice of the scientific inquiry in the 21th century. Within last four decades, computational experiment has become an important contributor to all scientific research programs. It is particular important for the solution of the research problems that are insoluble by traditional theoretical and experimental approaches, hazardous to study in the laboratory, or time consuming or expensive to solve by traditional means. Computational experiment includes several important ingredients: creating mathematical model, discretization, solvers, coding, verification and validation, visualization, analysis of the results, etc. In this talk we will describe some aspects of the modern numerical methods for high-speed, compressible, multi-physics, multi-material flows. We will address meshing issues, mimetic discretizations of equations of the Lagrangian gas dynamics and diffusion equation on general polygonal meshes, mesh adaptation strategies, methods for dealing with shocks, interface reconstruction needed for multi-material flows, closure models for multi-material cells, time discretizations, etc.

This review is based on following papers: paper [1] describes all main stages of arbitrary-Lagrangian-Eulerian methods for multi-material flows, and paper [2] describes mimetic finite difference method, which is used for most of the discretizations.

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

Evgeniy Romenski

(joint work with Galina Reshetova, Ilya Peshkov, Michael Dumbser)

A new approach, presented in [1]-[5], is discussed, which is based on the theory of Symmetric Hyperbolic Thermodynamically Compatible (SHTC) systems, for modeling a saturated deformable porous medium considered as a multiphase mixture. Many well-known equations of continuum mechanics are included in the class of SHTC systems. Moreover, the SHTC theory can be used as a tool for developing new correct mathematical models of complex media. A description and applications of this theory can be found in [6] and references therein.

We present a model that takes into account finite deformations of a porous medium saturated with a mixture of compressible liquids and gases. In general

the formulated SHTC model makes it possible to take into account the viscosity of saturating liquids and inelastic deformations of a porous skeleton. The governing PDEs satisfy the laws of nonequilibrium thermodynamics and form a symmetric hyperbolic system with curl involutions. Dissipative processes, such as equalization of phase pressures and interfacial friction, are taken into account by stiff algebraic source terms.

The structure of the governing PDEs, 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 number of numerical simulations are presented to demonstrate the capabilities of the model.

Simplification of the model for an elastic porous medium saturated with a single compressible fluid gives physically correct results close to those obtained using Biot's model generally accepted in geophysics. It should be noted that the Biot model is essentially linear, and we do not know its generalization to the case of finite deformations. The presented SHTC model, in our opinion, can serve as a basis for the development of new approaches to the study of nonlinear processes when considering finite deformations of saturated porous media of complex rheology.

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

François Dubois
(joint work with Filipa Caetano and Benjamin Graille)

We have presented an introduction of lattice Boltzmann schemes, with the first ideas of cellular automata on a square lattice [1], their extension to triangular lattices [2] and a spectacular numerical result proposed in [3]. The major characteristic of these discrete flows is the presence of Monte-Carlo noise. Then cellular automata have been replaced by various approximations of Boltzmann equation with discrete velocities. The simplest example [4] contains only two velocities.

The one-dimensional model with two velocities [5] is denoted by D1Q2 in the terminology of lattice Boltzmann schemes. It introduces a given velocity a, an equilibrium function $\mathbb{R} \ni u \longmapsto \Phi(u) \in \mathbb{R}$ and a small positive parameter ε:

$$\partial_t u + \partial_x v = 0 \,, \ \partial_t v + a^2 \, \partial_x u = \frac{1}{\varepsilon} \big(\Phi(u) - v \big) \,. \tag{1}$$

A formal Chapman-Enskog expansion at first order relative to ε conducts to a second order equivalent partial differential equation:

$$\partial_t u + \partial_x \Phi(u) - \varepsilon \, \partial_x \big((a^2 - \Phi'(u)^2) \, \partial_x u \big) = \mathrm{O}(\varepsilon^2) \,. \tag{2}$$

A rigorous proof of convergence is established in [6]. The discretisation with finite volume schemes leads to a convergent approach and this has been established in [7, 8].

For the system (1), the lattice Boltzmann scheme first consider the ordinary differential equation $\partial_t v = \frac{1}{\varepsilon} \big(\Phi(u) - v \big)$ and implement an explicit first order scheme during this collision step:

$$v_j^* = v_j^n + \frac{\Delta t}{\varepsilon} \, \big(\Phi(u_j^n) - v_j^n \big) \,. \tag{3}$$

The parameter $s \equiv \frac{\Delta t}{\varepsilon}$ is directly introduced as a given number in the numerical simulation. After this collision step, the density of particles $f_\pm^*$ are naturally associated to a diagonalized form of the system (1) and we have $\big(f_+^* \big)_j = \frac{1}{2} \big(u + \frac{v^*}{a} \big)_j$, $\big(f_-^* \big)_j = \frac{1}{2} \big(u - \frac{v^*}{a} \big)_j$. Then the propagation of the particles during one time step is written with an upwind scheme associated to a Courant number always identical to 1:

$$\big(f_+ \big)_j^{n+1} = \big(f_+^* \big)_{j-1} \,, \ \big(f_- \big)_j^{n+1} = \big(f_-^* \big)_{j+1} \,. \tag{4}$$

Finally the moments u and v at the new time step follow the simple relations $u_j^{n+1} = \big(f_+ \big)_j^{n+1} + \big(f_- \big)_j^{n+1}$ and $v_j^{n+1} = a \, \big[\big(f_+ \big)_j^{n+1} - \big(f_- \big)_j^{n+1} \big]$. Consistency of the numerical scheme (3)(4) with the system (1) is satisfied when $a = \frac{\Delta x}{\Delta t}$.

The previous D1Q2 scheme is generalized to a large number of DdQq stencils for d space dimensions and q discrete velocities. The principle is always to treat the collision with an explicit time scheme and the discrete advection with the exact scheme for a Courant number equal to unity. We refer to [9, 10, 11, 12, 13, 14] for major developments of lattice Boltzmann schemes.

The asymptotic analysis supposes typically that the ratio $\lambda \equiv \frac{\Delta x}{\Delta t}$ is fixed and that the relation parameter $s \equiv \frac{\Delta t}{\varepsilon}$ is also fixed. When the space and time steps tend to zero, the lattice Boltzmann scheme (3)(4) can be formally expanded and an equivalent partial differential equation is emerging. For the previous scheme, we obtain

$$\partial_t u + \partial_x \Phi(u) - \Delta t \left(\frac{1}{s} - \frac{1}{2}\right) \partial_x \big((a - \Phi'(u)^2)\, \partial_x u \big) = \mathrm{O}(\Delta t^2)\,. \tag{5}$$

This result was first obtained in [15] for cellular automata. It has been extended with the Taylor expansion method [16, 17, 18] to general nonlinear lattice Boltzmann schemes up to fourth order accuracy [19]. Observe in the relation (5) that for $s \simeq 2$, the asymptotic viscosity is drastically reduced in comparison with the expansion (2). In consequence, industrial applications at high Reynolds number are used in automotive industry [20] since 20 years and are in development for transonic aerodynamics [21].

Nevertheless, we have reported in [22, 23] an unexpected convergence previously observed in [17] for the heat equation when the time and space steps tend to zero with a fixed ratio $\lambda \equiv \frac{\Delta x}{\Delta t}$. The thermal diffusion coefficient evaluated with the Taylor expansion method $\mu \simeq \left(\frac{1}{s} - \frac{1}{2}\right) \lambda\, \Delta x$ remains constant and Δx tends to zero. Therefore, the parameter s tends also to zero and is no more fixed as supposed in the asymptotic expansion. The lattice Boltzmann equation remains stable, even if it is an explicit scheme with a ratio $\frac{\Delta t}{\Delta x^2}$ larger than 1. But it is no more consistent with the heat equation, and converges to a system of damped acoustics!

Finally, considering again the lattice Boltzmann scheme (3)(4), we can write it as a finite difference scheme:

$$\left\{ \begin{array}{l} \frac{u_j^{n+1} - u_j^n}{\Delta t} + \frac{v_{j+1}^n - v_{j-1}^n}{2\,\Delta x} - \frac{1}{2}\,\frac{\Delta x^2}{\Delta t}\,\frac{u_{j+1}^n - 2\,u_j^n + u_{j-1}^n}{\Delta x^2} \\ \qquad + \frac{s}{2\,\lambda\,\Delta t}\left((\Phi(u_{j+1}^n) - v_{j+1}^n) - (\Phi(u_{j-1}^n) - v_{j-1}^n) \right) = 0 \\ \frac{v_j^{n+1} - v_j^n}{\Delta t} + \lambda^2\,\frac{u_{j+1}^n - u_{j-1}^n}{2\,\Delta x} - \frac{1}{2}\,\frac{\Delta x^2}{\Delta t}\,\frac{v_{j+1}^n - 2\,v_j^n + v_{j-1}^n}{\Delta x^2} \\ \qquad - \frac{s}{2\,\Delta t}\left((\Phi(u_{j+1}^n) - v_{j+1}^n) + (\Phi(u_{j-1}^n) - v_{j-1}^n) \right) = 0\,. \end{array} \right. \tag{6}$$

In [24], we have proven the following convergence theorem. When $\lambda \equiv \frac{\Delta x}{\Delta t}$ is fixed and if the parameter $0 < s \leq 1$ is also fixed, the D1Q2 lattice Boltzmann scheme (3)(4) or (6) converges to the unique entropy solution of the scalar conservation law $\partial_t u + \partial_x \Phi(u) = 0$. The proof uses classical mathematical methods [7, 8] for establishing the convergence: L^∞ stability, total variation estimates, and discrete entropy inequalities.

The lattice Boltzmann schemes have proven their efficiency for a wide number of applications like isothermal flows, compressible flows with heat transfer, non-ideal fluids, multiphase and multi-component flows, microscale gas flows, soft-matter flows, *etc.* Last but not least, stability is one of the main remaining open questions.

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Hamiltonian mechanics leads to hyperbolic partial differential equations

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(joint work with M. Grmela, V. Klika, I. Peshkov, E. Romenskii, O. Kincl, O. Esen, D. Jou, M. La Mantia, P. Minakowski, and M. Sýkora)

We studied relations between Hamiltonian mechanics and hyperbolic quasilinear first-order partial differential equations. First, we recalled Hamiltonian continuum mechanics with dissipation, in the context of the General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) [5, 8, 7, 9]. Then, we showed that the framework of Symmetric Hyperbolic Thermodynamically Compatible equations (SHTC) [4, 12, 2, 11] is contained within GENERIC and that Hamiltonian mechanics can be used to generalize SHTC (in mixtures or superfluids [13]). In particular, the Hamiltonian structure of the equations can be used for proving their hyperbolicity. Finally, we have shown preliminary results on symplectic solvers for fluid mechanics and SHTC equations, using a variant of smoothed particle hydrodynamics (SPH) [6].

Within the GENERIC framework, evolution equations of any state variables $\mathbf{q}$ are composed of two parts, a reversible Hamiltonian part (mechanics) and an irreversible gradient part (thermodynamics),

$$\partial_t q^i = \{q^i, E\} + \frac{\partial \Xi}{\partial q_i^*}\Big|_{\mathbf{q}^* = \frac{\partial S}{\partial \mathbf{q}}}. \tag{1}$$

The reversible part is generated by a Poisson bracket $\{\bullet, \bullet\}$ and energy $E(\mathbf{q})$ while the irreversible by a dissipation potential $\Xi(\mathbf{q}, \mathbf{q}^*)$ and entropy $S(\mathbf{q})$. This framework contains many physical models like mechanics with friction, fluid mechanics, complex fluids, visco-elasto-plasticity, chemical kinetics, kinetic theory, or electrodynamics [9].

Let us now discuss in more detail the Riemannian and hyperbolic character of some Hamiltonian systems. When the Poisson bivector, $L^{i(\mathbf{r}),j(\mathbf{r}')} = \{q^i(\mathbf{r}), q^j(\mathbf{r}')\}$, depends only on Dirac $\delta(\mathbf{r})$ and its first derivatives, is in all the above mentioned applications of GENERIC, and when the energy is ultralocal, $E = \int e(\mathbf{q}) d\mathbf{r}$, then the resulting evolution equations represent a system of quasilinear partial differential equations,

$$\partial_t q^i = f^i_k \partial_x q^k, \quad \text{where} \quad f^i_k = g^{ij}(\mathbf{q}) \frac{\partial^2 e}{\partial q^j \partial q^k} + b^{ij}_k \frac{\partial e}{\partial q^j}. \tag{2}$$

Here, g^{ij} is a symmetric tensor field that represents an inverse metric, for instance $g^{ij} = \begin{pmatrix} 0 & -\rho \\ -\rho & -2m \end{pmatrix}$ in the case of one-dimensional hydrodynamics with state variables $\mathbf{q} = (\rho, m)$ (density and momentum density). Dubrovin and Novikov showed [1], moreover, that if the metric is non-denenerate, $\det g^{ij} \neq 0$, then: (i) $b^{ij}_k = -g^{is}\Gamma^j_{sk}$, which gives a Levi-civita connection ∇ with Christoffel symbols

Γ^j_{sk}, (ii) g^{ij} and ∇ are compatible, (iii) ∇ is curvature-free and torsion-free, (iv) and thus $f^i_k = g^{ij}\nabla_j\nabla_k e$. The system of equation (2) then becomes

$$\partial_t q^i = g^{is}\nabla_s\nabla_k e\partial_x q^k. \tag{3}$$

Similarly as in the Godunov's theorem [3], we now go to the Legendre transform, $p_i = \frac{\partial e}{\partial q^i}$, $L = -e + q^i p_i$, and $q^i = \frac{\partial L}{\partial p_i}$. The Hamiltonian system of hydrodynamic type (3) then gains the symmetric hyperbolic form,

$$H_L\partial_t\mathbf{p} - \mathbf{g}\partial_x\mathbf{p} = 0, \tag{4}$$

where Hessian H_L is symmetric positive definite for convex energies e.

Unlike the Godunov theorem, this approach can prove symmetric hyperbolicity also when the equations are not conservation laws. On the other hand, the non-degeneracy of the metric is a rather restrictive property of the system. This approach towards symmetric hyperbolicity of the equations works for instance in the case of one-dimensional binary mixtures with state variables $\mathbf{q} = (\rho_1, m_1, \rho_2, m_2)$, which are not in the conservative form if $\frac{\partial^2 e}{\partial\rho_1\partial\rho_2} \neq 0$ [10], and thus it provides an alternative to Godunov's theorem.[1]

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