Kinetic schemes for compressible flows with phase transition

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Outlines

Motivation: kinetic approximations of conservation laws allow to design very efficient high order schemes. Apply it to multiphase flows.

Kinetic relaxation and over-relaxation

Equivalent PDE

Application to multiphase flows

Kinetic relaxation in higher dimensions

Kinetic relaxation and over-relaxation

Relaxation of hyperbolic systems

- Hyperbolic system with unknown $\mathrm{u}(x,t) \in \mathbb{R}^m$:

$$\partial_t \mathrm{u} + \partial_x \mathrm{f}(\mathrm{u}) = 0.$$

LHS: non-linear equations ☹; RHS: zero ☺.

- Approximation by Jin-Xin[1] relaxation ($\lambda > 0$, $\varepsilon \to 0^+$)

$$\partial_t \mathrm{u} + \partial_x \mathrm{z} = 0, \tag{1}$$

$$\partial_t \mathrm{z} + \lambda^2 \partial_x \mathrm{u} = \mu, \tag{2}$$

where

$$\mu = \frac{1}{\varepsilon}(\mathrm{f}(\mathrm{u}) - \mathrm{z}).$$

LHS: linear system with constant coefficients ☺; RHS: non-linear coupling ☹.

[1] **jin1995relaxation**.

Over-relaxation

Let's do splitting. For a rigorous formulation, introduce the Dirac comb:

$$\Psi(t) = \sum_{i\in\mathbb{Z}} \delta(t - i\Delta t).$$

Jin-Xin relaxation is replaced in practice by

$$\partial_t \mathsf{u} + \partial_x \mathsf{z} = 0, \quad (3)$$

$$\partial_t \mathsf{z} + \lambda^2 \partial_x \mathsf{u} = \mu, \quad (4)$$

with

$$\mu(x,t) = \theta\Psi(t)\left(\mathsf{f}(\mathsf{u}(x,t)) - \mathsf{z}(x,t^-)\right), \quad \theta \in [1,2].$$

In other words, at times $t = i\Delta t$, z has jumps in time and:

$$\mathsf{z}(x,t^+) = \theta \mathsf{f}(\mathsf{u}(x,t)) + (1-\theta)\mathsf{z}(x,t^-).$$

If the relaxation parameter $\theta = 1$, we recover the first order splitting.
The **over-relaxation** corresponds to $\theta = 2$.

explicit, CFL-less Kinetic interpretation

We can diagonalize the linear hyperbolic operator. For this, consider the change of variables

$$\mathsf{k}^+ = \frac{\mathsf{u}}{2} + \frac{\mathsf{z}}{2\lambda}, \quad \mathsf{k}^- = \frac{\mathsf{u}}{2} - \frac{\mathsf{z}}{2\lambda}.$$

$$\mathsf{u} = \mathsf{k}^+ + \mathsf{k}^-, \quad \mathsf{z} = \lambda \mathsf{k}^+ - \lambda \mathsf{k}^-.$$

Then

$$\partial_t \mathsf{k}^+ + \lambda \partial_x \mathsf{k}^+ = \mathsf{r}^+, \quad \partial_t \mathsf{k}^- - \lambda \partial_x \mathsf{k}^- = \mathsf{r}^-,$$

where

$$\mathsf{r}^\pm(x,t) = \theta \Psi(t) \left(\mathsf{k}^{eq,\pm}(\mathsf{u}(x,t^-)) - \mathsf{k}^\pm(x,t^-) \right)$$

and the "Maxwellian" states $\mathsf{k}^{eq,\pm}$ are given by

$$\mathsf{k}^{eq,\pm}(\mathsf{u}) = \frac{\mathsf{u}}{2} \pm \frac{\mathsf{f}(\mathsf{u})}{2\lambda}.$$

Most of the time, the kinetic variables k^+ and k^- satisfy free transport equations at velocity $\pm\lambda$, with relaxation to equilibrium at each time step.

Equivalent PDE

Oscillations of the flux error

We consider the case $\theta = 2$.

- Let us introduce the "flux error"

$$\mathrm{y} := \mathrm{z} - \mathrm{f}(\mathrm{u}).$$

- At time $t = i\Delta t$, we see that

$$\mathrm{y}(x, t^+) = -\mathrm{y}(x, t^-).$$

  Therefore y oscillates around 0 at a frequency $1/\Delta t$.

- For the analysis, it is better to consider the solution only at even (or only at odd) times steps $t = 2i\Delta t$.

Equivalent PDE analysis

We can prove the following result (more rigorous formulation exists[2]).
Theorem: if the solution of the over-relaxation scheme is considered at even time steps, then, up to second order terms in Δt, its equivalent equation in (u,y) is the following hyperbolic system of conservation laws

$$\begin{aligned} \partial_t \mathrm{u} + \partial_x \mathrm{f}(\mathrm{u}) &= 0, \\ \partial_t \mathrm{y} - \mathrm{f}'(\mathrm{u}) \partial_x \mathrm{y} &= 0. \end{aligned}$$

Remarks:

- u satisfies the expected conservative system at order $O(\Delta t^2)$.
- y satisfies a non-conservative equation.
- There is no assumption on the smallness of y at the initial time.
- The waves for u and y move in opposite directions.

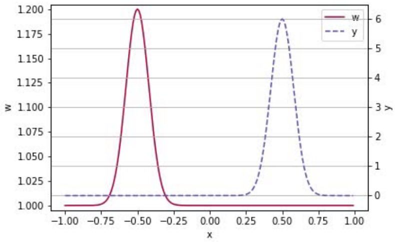
[2] **drui2019analysis**.

Numerical results

- Isothermal Euler equations

$$u = (\rho, \rho u)^T, \quad f(u) = (\rho u, \rho u^2 + c^2 \rho).$$

- Smooth initial data with a bump. Supersonic flow moving rightward ($0 < \lambda_1 = u - c < \lambda_2 = u + c$). Non-physical initial value of $y \neq 0$.
- Transport equations solved with an exact characteristic scheme (Lattice-Boltzmann Method).
- We plot ρ and the first component of y at even time steps. We clearly observe the opposite propagation of the waves.



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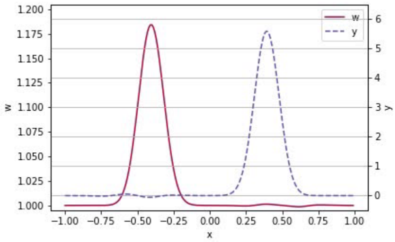

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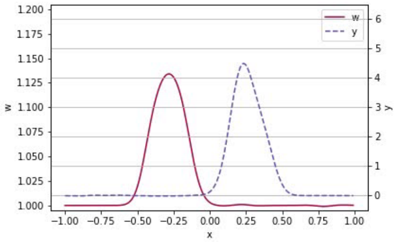

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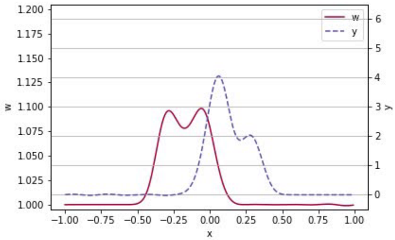

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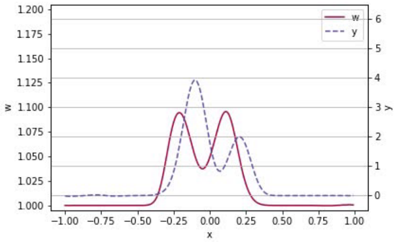

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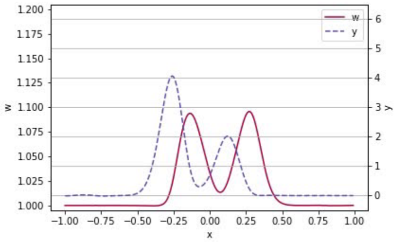

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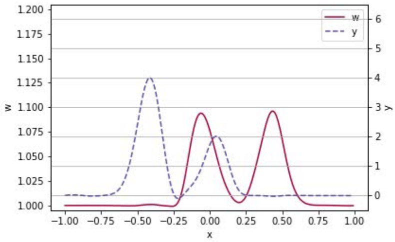

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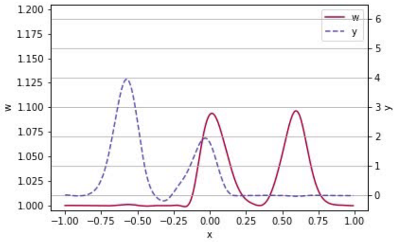

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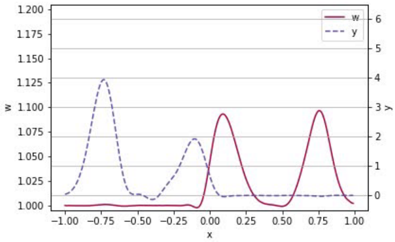


Application to multiphase flows

1D flow with phase transition

- Mixture of water and air.
- Unknowns: density ρ, velocity v, pressure p, internal energy ε and mass fraction of the inert gas φ.
- Pressure law:

$$p = p(\rho, \varepsilon, \varphi).$$

- Total energy: $E = \rho\varepsilon + \frac{1}{2}\rho v^2$.
- The equations are $\partial_t \mathrm{u} + \partial_x \mathrm{f}(\mathrm{u}) = 0$ with

$$\mathrm{u} = (\rho, \rho v, \rho E, \rho\varphi)^\intercal, \quad \mathrm{f}(\mathrm{u}) = (\rho v, \rho v^2 + p, (\rho E + p)v, \rho v \varphi)^\intercal.$$

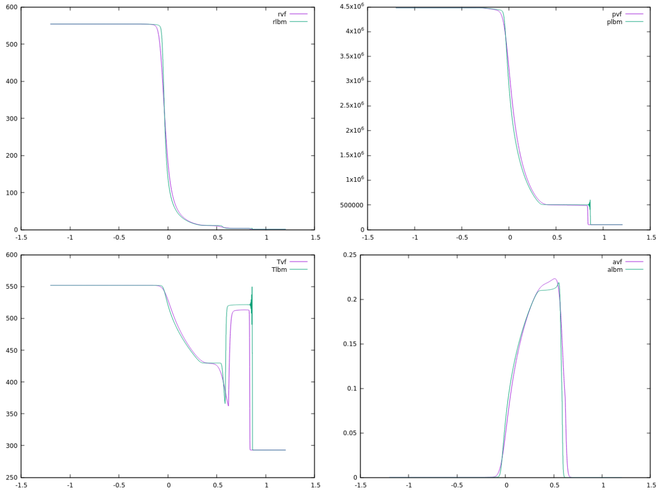
The pressure is obtained from a physical thermodynamical construction that ensures the existence of a convex entropy and a convex hyperbolicity domain.

Numerical results

	liquid (L)	air (R)
ρ	554.09	1.186245
ε	1161999.729	210749.040
φ	10^{-6}	$1-10^{-6}$

Table: Vapor explosion Riemann problem parameters.

Numerical results



Top left: density, top right: pressure, bottom left: temperature, bottom right: vapor mass fraction. Comparison between the Finite Volume and Lattice Boltzmann Method with $\omega = 1.9$ on a mesh with 2000 cells.

Kinetic relaxation in higher dimensions

Kinetic model in higher dimensions[3,4]

- Vectorial kinetic equation

$$\partial_t \mathrm{k} + \sum_{i=1}^{D} \mathrm{V}^i \partial_i \mathrm{k} = \frac{1}{\tau}(\mathrm{k}^{eq}(\mathrm{k}) - \mathrm{k}). \tag{5}$$

  $\mathrm{k}(\mathrm{x}, t) \in \mathbb{R}^n$, $\mathrm{x} \in \mathbb{R}^D$.

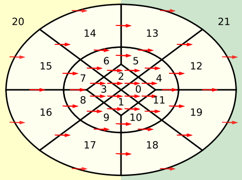
- The matrices V^i, $1 \leq i \leq D$ are **diagonal** and **constant**.
- $\mathrm{u} = \mathrm{Pk}$ where P is a constant $m \times n$ matrix, $m < n$.
- The equilibrium distribution $\mathrm{k}^{eq}(\mathrm{k})$ is such that $\mathrm{Pk} = \mathrm{Pk}^{eq}(\mathrm{k})$.
- When $\tau \to 0$, approximation of $\partial_t \mathrm{u} + \sum_{i=1}^{D} \partial_i \mathrm{f}^i(\mathrm{u}) = 0$, where the flux is given by $\mathrm{f}^i(\mathrm{u}) = \mathrm{PV}^i \mathrm{k}^{eq}(\mathrm{k})$.

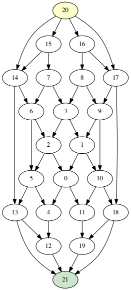
[3] **bouchut1999construction**.

[4] **aregba2000discrete**.

CFL-less kinetic DG scheme

- On unstructured meshes, it is easy to solve the kinetic transport equations with an implicit upwind Discontinuous Galerkin scheme.
- In practice, the scheme is **explicit** if the cells are visited in the good order.





- In this way we obtain **explicit unconditionnaly stable** schemes !

CFL-less kinetic DG scheme

Example: Maxwell equations. Comparison RK3 and CFL-less scheme.

Onde plane de fréquence $\nu = 0.5$

Méthode	CFL	iter.	Δt	$\|\|\mathbf{u} - \mathbf{u}^{ex}\|\|_{L^2}$	CPU (s)	ordre σ
D3Q4	96.69	53	$1.86 \cdot 10^{-2}$	$4.10 \cdot 10^{-4}$	10.67	—
D3Q4	48.37	106	$9.31 \cdot 10^{-3}$	$1.09 \cdot 10^{-4}$	19.2	1.92
D3Q4	24.17	212	$4.66 \cdot 10^{-3}$	$3.14 \cdot 10^{-5}$	38.86	1.79
D3Q4	12.09	424	$2.33 \cdot 10^{-3}$	$1.31 \cdot 10^{-5}$	80.43	1.26
D3Q4	6.04	848	$1.16 \cdot 10^{-3}$	$1.01 \cdot 10^{-5}$	148.7	0.37
RK3	1.04	4,935	$2.00 \cdot 10^{-4}$	$9.47 \cdot 10^{-6}$	601.53	—
RK3	0.52	9,870	$1.00 \cdot 10^{-4}$	$9.47 \cdot 10^{-6}$	1,192.39	—

Temps moyen par itération :

- **D3Q4** $\simeq$ $0.17s$
- **RK3** $\simeq$ $0.12s$

Paramètres :

- Maillages : `torus_in_cube.msh`
- Nb. elem. : 18,731
- Nb. inc. : 4,495,440
- h : 0.000193
- t : 1
- **CPU** : `Intel(R) Core(TM) i7-5820K CPU @ 3.30GHz (12 cores)`

CFL-less kinetic DG scheme

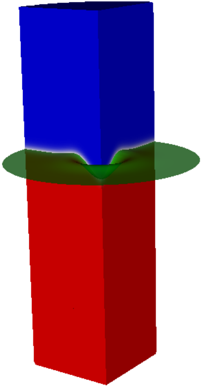
Further improvements

- High order in space and time with palindromic splitting[5];
- Easy parallelization, with a task-based approach and StarPU runtime system[6];
- Applications to: compressible flows, MHD, two-phase flow, *etc.*[7]

[5] **hairer2006geometric**.
[6] **badwaik2018task**.
[7] **COULETTE2019**.

Thanks for your attention !

Rayleigh-Taylor instability. Two immiscible fluids with gravity. CFL=10.



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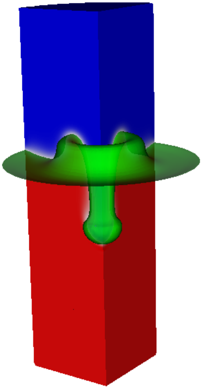

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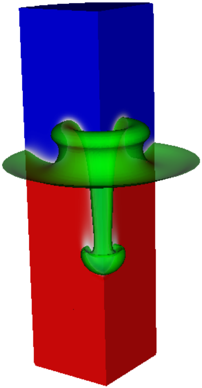

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