Kinetic schemes for compressible flows with phase transition
Philippe Helluy

University of Strasbourg, Inria Tonus

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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 $u(x, t) \in \mathbb{R}^m$:

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

\text{LHS: non-linear equations ☹; RHS: zero ☺.}

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

$$\partial_t u + \partial_x z = 0, \quad (1)$$

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

where

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

\text{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

$$\partial_t u + \partial_x z = 0,$$
$$\partial_t z + \lambda^2 \partial_x u = \mu,$$

with

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

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

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

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

\[
\begin{align*}
k^+ &= \frac{u}{2} + \frac{z}{2\lambda}, & k^- &= \frac{u}{2} - \frac{z}{2\lambda}, \\
u &= k^+ + k^-, & z &= \lambda k^+ - \lambda k^-.
\end{align*}
\]

Then

\[
\begin{align*}
\partial_t k^+ + \lambda \partial_x k^+ &= r^+, & \partial_t k^- - \lambda \partial_x k^- &= r^-,
\end{align*}
\]

where

\[
r^\pm(x, t) = \theta \Psi(t) (k^{eq,\pm}(u(x, t^-)) - k^\pm(x, t^-))
\]

and the “Maxwellian” states \(k^{eq,\pm}\) are given by

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

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”
  
  \[ y := z - f(u). \]

- At time $t = i\Delta t$, we see that
  
  \[ y(x, t^+) = -y(x, t^-). \]

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 \(\Delta t\), its equivalent equation in \((u, y)\) is the following hyperbolic system of conservation laws

\[
\begin{align*}
\partial_t u + \partial_x f(u) &= 0, \\
\partial_t y - f'(u)\partial_x y &= 0.
\end{align*}
\]

**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.

\(^2\text{drui2019analysis.}\)
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 \(\rho\) and the first component of \(y\) at even time steps. We clearly observe the opposite propagation of the waves.
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Application to multiphase flows
Mixture of water and air.

Unknowns: density $\rho$, velocity $v$, pressure $p$, internal energy $\varepsilon$ and mass fraction of the inert gas $\phi$.

Pressure law:

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

Total energy:

$$E = \rho \varepsilon + \frac{1}{2} \rho v^2.$$

The equations are $\partial_t u + \partial_x f(u) = 0$ with

$$u = (\rho, \rho v, \rho E, \rho \phi)^T, \quad f(u) = (\rho v, \rho v^2 + p, (\rho E + p)v, \rho v \phi)^T.$$

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

<table>
<thead>
<tr>
<th></th>
<th>liquid (L)</th>
<th>air (R)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \rho )</td>
<td>554.09</td>
<td>1.186245</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>1161999.729</td>
<td>210749.040</td>
</tr>
<tr>
<td>( \varphi )</td>
<td>( 10^{-6} )</td>
<td>( 1 - 10^{-6} )</td>
</tr>
</tbody>
</table>

**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\textsuperscript{3,4}

- Vectorial kinetic equation

\begin{equation}
\partial_t k + \sum_{i=1}^{D} V^i \partial_i k = \frac{1}{\tau} (k^{eq}(k) - k).
\end{equation}

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

- The matrices \(V^i, 1 \leq i \leq D\) are \textbf{diagonal} and \textbf{constant}.

- \(u = Pk\) where \(P\) is a constant \(m \times n\) matrix, \(m < n.\)

- The equilibrium distribution \(k^{eq}(k)\) is such that \(Pk = Pk^{eq}(k).\)

- When \(\tau \to 0\), approximation of \(\partial_t u + \sum_{i=1}^{D} \partial_i f^i(u) = 0\), where the flux is given by \(f^i(u) = PV^i k^{eq}(k)\).

\textsuperscript{3}bouchut1999construction.  
\textsuperscript{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 unconditionally 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. | $\Delta t$ | $||u - u^{ex}||_{L^2}$ | CPU (s) | ordre $\sigma$ |
|---------|------|-------|-----------|-----------------|--------|----------|
| 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 $\approx 0.17s$
- RK3 $\approx 0.12s$

**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)
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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