A fourth-order entropic kinetic scheme

Thomas Bellotti, Philippe Helluy, Laurent Navoret

Université de Strasbourg, IRMA CNRS

ProHyp workshop, Trento, April 2024
The kinetic representation of conservation laws is a useful tool. Some applications:

- Very efficient schemes on structured grids (Lattice Boltzmann Method, LBM).
- CFL-less explicit schemes on structured or unstructured grids.

In this talk we present an extension of the LBM to fourth-order accuracy that respects entropy dissipation.

Outline:

Kinetic representation

Entropy stability

Numerical results
Kinetic representation
Vectorial kinetic model

Abstract kinetic BGK model

\[ \partial_t F + V \cdot \partial_x F = \frac{1}{\varepsilon} (F^{eq} - F), \]  \hspace{1cm} (1)

where

- Vector distribution: \( F(\mathbf{x}, t) \in \mathbb{R}^n \), space variable: \( \mathbf{x} \in \mathbb{R} \), time variable: \( t \).
- \( V \) is a constant diagonal matrix.
- \( F^{eq} \) is the equilibrium distribution function, \( \varepsilon \) is a small positive parameter.

\[1^{[Bouchut(1999), Aregba-Driollet and Natalini(2000)]}\]
Macroscopic model

We consider a constant invertible $n \times n$ matrix $M$ of the form

$$M = \begin{pmatrix} P \\ R \end{pmatrix},$$

where $P$ is of size $m \times n$ and $R$ is of size $(n - m) \times n$. The macroscopic conserved variables are

$$W = PF.$$

We impose that $F^{eq}$ depends only on $W = PF$ and that

$$W = PF = PF^{eq}(W).$$

We also introduce the “flux error”, which vanishes when $F = F^{eq}$:

$$Y = RF - RF^{eq}.$$
When the relaxation parameter $\varepsilon \to 0^+$, the macroscopic data $W$ formally satisfies the system of conservation laws

$$\partial_t W + \partial_x Q(W) = 0,$$

where the flux $Q$ is given by

$$Q(W) = PVF^{eq}(W).$$

Thus the kinetic BGK model (1) is an approximation of (2).
Formal proof

Multiply the BGK equation by $P$ on the left, and use the relation $PF = PF^{eq}$:

$$\partial_t PF + \partial_x PVF = \frac{1}{\varepsilon}(PF - PF^{eq}) = 0.$$ 

Because $W = PF$ and $F \simeq F^{eq}$, we get

$$\partial_t W + \partial_x PVF^{eq}(W) = \partial_t W + \partial_x Q(W) \simeq 0.$$ 

This proof is purely algebraic, without consideration about: hyperbolicity, entropy, H-principle, stability, etc. For a system of $m$ equations in space dimension $d$ it is always possible to find a kinetic representation of size $n = m(d + 1)$. 
Minimal example: Jin-Xin$^2$

D1Q2 kinetic representation of a system of $m$ conservation laws

$$\partial_t W + \partial_x Q(W) = 0.$$ 

We take $n = 2m$ and

$$V = \begin{pmatrix} -\lambda I & 0 \\ 0 & \lambda I \end{pmatrix}, \quad M = \begin{pmatrix} I & I \\ -\lambda I & \lambda I \end{pmatrix}, \quad F^{eq} = \begin{pmatrix} W/2 - Q(W)/2\lambda \\ W/2 + Q(W)/2\lambda \end{pmatrix}.$$ 

The velocity $\lambda > 0$ is a large enough constant for ensuring stability. For simplicity, but without loss of generality, we consider only this model in the following. We also set

$$F = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix}, \quad F_k \in \mathbb{R}^m.$$ 

Note that $Y = -\lambda F_1 + \lambda F_2 - Q(W)$ and it is indeed a “flux error”.

$^2$[Jin and Xin(1995)]
1. Start with $W(\cdot, 0)$. Construct a kinetic vector $F(\cdot, 0)$ such that $W = PF$.

2. Solve the free transport equations $\partial_t F + V \cdot \nabla F = 0$ for a duration of $\Delta t$. Because $V = \text{diag}(-\lambda I, \lambda I)$, explicit formula

$$F_1(X, \Delta t^-) = F_1(X+\lambda \Delta t, 0), \quad F_2(X, \Delta t^-) = F_2(X-\lambda \Delta t, 0).$$

3. Define

$$W(\cdot, \Delta t) = PF(\cdot, \Delta t^-).$$

4. Apply a relaxation towards equilibrium (this emulates $\partial_t F = (F^{eq} - F)/\varepsilon$)

$$F(\cdot, \Delta t^+) = \omega F^{eq}(W(\cdot, \Delta t)) + (1 - \omega)F(\cdot, \Delta t^-).$$

Interesting cases: $\omega = 1$ (first order splitting), $\omega = 2$ (second order splitting).
LBM in the \((W, Y)\) variables

We rewrite the LBM in the \((W, Y)\) variables:

- **Transport step**

\[
\begin{pmatrix}
W(\cdot, \Delta t) \\
Y(\cdot, \Delta t^-)
\end{pmatrix} = \mathcal{T}(\Delta t) \begin{pmatrix}
W(\cdot, 0) \\
Y(\cdot, 0^+)
\end{pmatrix}.
\]

- **Relaxation step**

\[
\begin{pmatrix}
W(\cdot, \Delta t) \\
Y(\cdot, \Delta t^+)
\end{pmatrix} = \mathcal{R}_\omega \begin{pmatrix}
W(\cdot, \Delta t) \\
Y(\cdot, \Delta t^-)
\end{pmatrix} = \begin{pmatrix}
W(\cdot, \Delta t) \\
(1 - \omega)Y(\cdot, \Delta t^-)
\end{pmatrix}.
\]

The application of one time-step of the LBM then reads, in the operator form,

\[
\begin{pmatrix}
W \\
Y
\end{pmatrix} \leftarrow \mathcal{B}(\Delta t) \begin{pmatrix}
W \\
Y
\end{pmatrix}, \quad \mathcal{B}(\Delta t) = \underbrace{\mathcal{R}_\omega}_{\text{relax.}} \underbrace{\mathcal{T}(\Delta t)}_{\text{transport}}.
\]
Properties of the relaxation

For $\omega = 2$, the relaxation operator is an involution:

$$R_2 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad R_2^2 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}.$$ 

It is reversible ($\simeq$ entropy conservative).

For $\omega = 1$, it is a projection:

$$R_1 = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad R_1^2 = R_1,$$

and thus not reversible ($\simeq$ entropy dissipative).
Time-symmetric correction

The LBM scheme is second order in time. It is not obvious because it does not look like a Strang splitting algorithm\(^3\). We can write a time-symmetric version of the basic brick \( B \):

\[ B(\Delta t) = T\left( \frac{\Delta t}{4} \right) R_\omega T\left( \frac{\Delta t}{2} \right) R_\omega T\left( \frac{\Delta t}{4} \right). \]

Note that the transport step remains a shift algorithm if one takes \( \Delta x = \lambda \Delta t/4 \), for instance. Then we have, for \( \omega = 2 \):

\[ B(-\Delta t) = B(\Delta t)^{-1}, \quad B(0) = I. \]

Time-symmetry expresses the time reversibility of the scheme. This is not unreasonable as long as we are interested in smooth solutions. It ensures second order accuracy of the time integration\(^4\).

\(^3\)[Dubois(2008), Dellar(2013)]
\(^4\)[McLachlan and Quispel(2002)]
For $\omega = 2$, by Taylor expansions in $\Delta t$, we can compute the formal equivalent equation of the time-symmetric LBM scheme. We get

$$\partial_t \begin{pmatrix} W \\ Y \end{pmatrix} + \begin{pmatrix} Q'(W) & 0 \\ 0 & -Q'(W) \end{pmatrix} \partial_x \begin{pmatrix} W \\ Y \end{pmatrix} = O(\Delta t^2).$$

- Up to second order, the evolution of $W$ and $Y$ are uncoupled.
- The flux error $Y$ does not need to be small.
- The waves for $W$ and $Y$ move in opposite directions.
Higher order by composition

We look for a higher order splitting scheme of the form

\[ \mathcal{H}(\Delta t) = B(\alpha \Delta t)^k B(\beta \Delta t) B(\alpha \Delta t)^k. \]

This palindromic composition scheme is fourth order, provided that\(^5\)

\[ 2k\alpha + \beta = 1, \quad 2k\alpha^3 + \beta^3 = 0. \] (3)

Some worries:

▷ if \( \alpha > 0 \) then \( \beta < 0 \) (negative time-stepping).

▷ For most choices of the integer \( k \), \( \alpha/\beta \) is not rational and thus the LBM trick (exact shifts on a structured grid) does not apply.

But:

▷ negative time-stepping is not a problem, because of time reversibility in the smooth case.

▷ If you take \( k = 4 \), then \( \alpha = 1/6, \beta = -1/3 \) is a rational solution of (3) !

\(^5\)\text{[McLachlan and Quispel(2002)]}
Fourth-order LBM strategy

4th-order LBM $\mathcal{H}(\Delta t)$

2nd-order LBM

Classical LBM: 24 steps, fourth-order scheme: 32 steps. The cost is 30% higher for advancing of $\Delta t$. Low-storage: only one time-step of the solution needs to be stored in memory.
Entropy stability
Kinetic entropies\(^6\)

Lax entropy
\[
\partial_t U(W) + \partial_x G(W) \leq 0,
\]
\(U\) convex, \(D_W U(W) D_W Q(W) = D_W G(W)\).

Find kinetic entropies \(U_k\) satisfying
\[
U(W) = \min_{PF=W} \sum_k U_k(F_k) = \sum_k U_k(F^{eq}_k(W)).
\]

The sum of the kinetic entropies can be expressed as a function of \((W, Y)\)
\[
\Sigma(W, Y) = \sum_k U_k(F_k),
\]
The equilibrium corresponds to \(Y = 0\), and \(\Sigma(W, 0) = U(W)\).

\(^6\)[Bouchut(1999), Aregba-Driollet and Natalini(2000)]
Linear case

Simple example: D1Q2 with $Q(W) = cW$ (linear transport). We can take $U(W) = W^2/2$.

$$U_1(F_1) = \frac{\lambda}{\lambda - c} (F_1)^2, \quad U_2(F_2) = \frac{\lambda}{\lambda + c} (F_2)^2.$$

$$\Sigma(W, Y) = \frac{W^2}{2} + \frac{Y^2}{2(\lambda^2 - c^2)}.$$

The convexity of the kinetic entropies is equivalent to the sub-characteristic condition

$$\lambda \geq |c|.$$

For a general non-linear system, the kinetic entropies can be found with Legendre transform calculations$^7$.

$^7$[Guillon et al.(2023)Guillon, Hélie, and Helluy]
Time-symmetric entropy conservative scheme

In the transport step, the kinetic entropies are separately conserved because

$$\partial_t U_k(F_k) + V_k \partial_x U_k(F_k) = 0.$$  

But for $\omega = 2$, the relaxation step does not preserve entropy in the non-linear case.
Fix: search the value $\omega(W, Y) \simeq 2$ such that

$$\sum_k U_k(F_k) = \sum_k U_k(F'_k), \quad F'_k = \omega F_{k eq} + (1 - \omega) F_k.$$  

In the $(W, Y)$ variables, this reads

$$\Sigma(W, Y) = \Sigma(W, (1 - \omega(W, Y)) Y).$$
Entropy conservation

In the non-linear case the entropy isolines are no more symmetric with respect to \( Y = 0 \). But with the above fix we recover entropy conservation. The resulting scheme is still time-symmetric because if

\[
\mathcal{R}_\omega(W, Y) (W, Y) = (W', Y')
\]

then

\[
\mathcal{R}_\omega(W', Y') (W', Y') = (W, Y).
\]
Numerical results
Alternative scheme

The fourth order scheme $\mathcal{B}$ is a sort of ideal entropy preserving scheme. In shocks waves it will produce terrible oscillations. But we can mix projections on equilibrium $\mathcal{R}_1$ with entropy conservative relaxations $\mathcal{R}_\omega(W,Y)$. We tested several strategies. We found the following choice to be excellent: we just modify the basic brick with a final projection onto equilibrium

$$
\mathcal{B}(\Delta t) = \mathcal{R}_1 \mathcal{T}(\frac{\Delta t}{4}) \mathcal{R}_\omega \mathcal{T}(\frac{\Delta t}{2}) \mathcal{R}_\omega \mathcal{T}(\frac{\Delta t}{4}).
$$

And take, as before

$$
\mathcal{H}(\Delta t) = \mathcal{B}(\frac{\Delta t}{6})^4 \mathcal{B}(\frac{-\Delta t}{3}) \mathcal{B}(\frac{\Delta t}{6})^4.
$$

This scheme remains fourth-order and entropy dissipative. More details in\(^8\).

\(^8\)[Bellotti et al.(2024)Bellotti, Helluy, and Navoret]
The test is done with the Burgers equation.

<table>
<thead>
<tr>
<th>$\Delta x$</th>
<th>Scheme 0</th>
<th>Scheme 1</th>
<th>Scheme 2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$L^2$ error</td>
<td>order</td>
<td>$L^2$ error</td>
</tr>
<tr>
<td>2.000E-03</td>
<td>8.592E-05</td>
<td>3.370E-06</td>
<td>3.374E-06</td>
</tr>
<tr>
<td>1.250E-03</td>
<td>3.358E-05</td>
<td>1.552E-06</td>
<td>1.551E-06</td>
</tr>
<tr>
<td>7.813E-04</td>
<td>1.404E-05</td>
<td>1.742E-07</td>
<td>1.742E-07</td>
</tr>
<tr>
<td>4.883E-04</td>
<td>5.494E-05</td>
<td>3.365E-08</td>
<td>3.365E-08</td>
</tr>
<tr>
<td>3.053E-04</td>
<td>2.160E-06</td>
<td>5.184E-09</td>
<td>5.184E-09</td>
</tr>
</tbody>
</table>

Scheme 0: second order LBM
Scheme 1: fourth-order time-symmetric LBM
Scheme 2: fourth-order with periodic projections
Stability tests

We check the non-linear stability of the first scheme with $\omega = 2$ and with the $\omega = \omega(W, Y)$ ensuring entropy conservation. This test is done with shallow water equations.
2D computations

Euler equations. 2D Lax Riemann problem
Conclusion

- Fourth-order LBM for hyperbolic conservation laws.
- Full entropy stability analysis.
- Ongoing work: boundary conditions.
Bibliography I

URL https://doi.org/10.1137/s0036142998343075.

URL https://hal.science/hal-04510582.

URL https://doi.org/10.1023%2Fa%3A1004525427365.


URL https://hal.science/hal-03986533.