A fourth-order entropic kinetic scheme

Thomas Bellotti, Philippe Helluy, Laurent Navoret

Université de Strasbourg, IRMA CNRS

ProHyp workshop, Trento, April 2024

Contents

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[1]

Abstract kinetic BGK model

$$\partial_t F + V \cdot \partial_x F = \frac{1}{\varepsilon}(F^{eq} - F), \tag{1}$$

where

- Vector distribution: $F(x, t) \in \mathbb{R}^n$, space variable: $x \in \mathbb{R}$, time variable: t.
- V is a constant **diagonal** matrix.
- F^{eq} is the equilibrium distribution function, ε 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 $F = F^{eq}$:

$$Y = RF - RF^{eq}.$$

System of conservation laws

When the relaxation parameter $\varepsilon \to 0^+$, the macroscopic data W formally satisfies the system of conservation laws

$$\partial_t W + \partial_x Q(W) = 0, \tag{2}$$

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

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

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)]

Lattice Boltzmann Method (LBM)

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 Δt. Because $V = \mathrm{diag}(-\lambda I, \lambda I)$, 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:

$$\mathcal{R}_2 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \mathcal{R}_2^2 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix}.$$

It is reversible ($\simeq$ entropy conservative).
For $\omega = 1$, it is a projection:

$$\mathcal{R}_1 = \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathcal{R}_1^2 = \mathcal{R}_1,$$

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 $\mathcal{B}$:

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

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

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

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)]

Equivalent equation

For $\omega = 2$, by Taylor expansions in Δt, 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

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

This palindromic composition scheme is fourth order, provided that[5]

$$2k\alpha + \beta = 1, \quad 2k\alpha^3 + \beta^3 = 0. \tag{3}$$

Some worries:

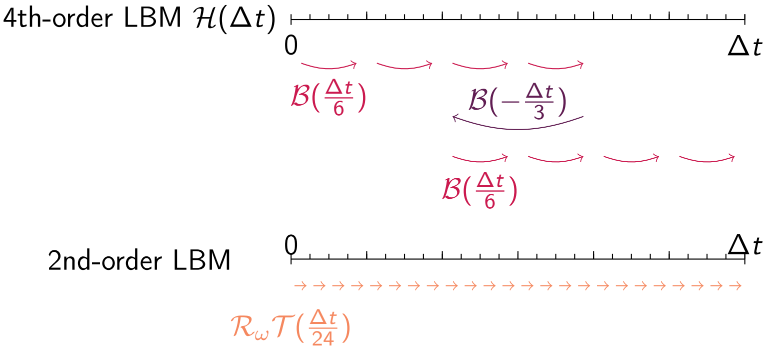
- if $\alpha > 0$ then $\beta < 0$ (negative time-stepping).
- For most choices of the integer k, α/β is not rational and thus the LBM trick (exact shifts on a structured grid) does not apply.

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] [McLachlan and Quispel(2002)]

Fourth-order LBM strategy



Classical LBM: 24 steps, fourth-order scheme: 32 steps. The cost is 30% higher for advancing of Δt. Low-storage: only one time-step of the solution needs to be stored in memory.

Entropy stability

Kinetic entropies[6]

Lax entropy

$$\partial_t U(W) + \partial_x G(W) \leq 0,$$

$$U \text{ convex}, \quad D_W U(W) D_W Q(W) = D_W G(W).$$

Find kinetic entropies U_k satisfying

$$U(W) = \min_{PF=W} \sum_k U_k(F_k) = \sum_k U_k(F_k^{eq}(W)).$$

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

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

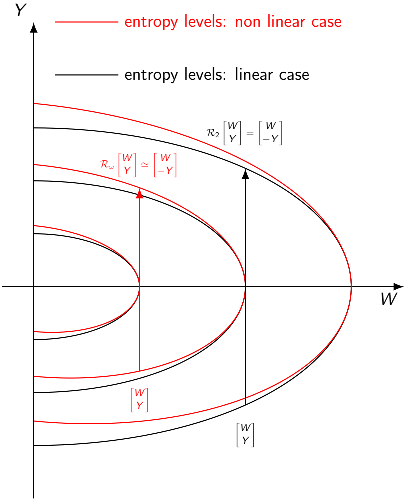
But for $\omega = 2$, the relaxation step does not preserve entropy in the non-linear case.
Fix: search the value $\omega(W, Y) \simeq 2$ such that

$$\sum_k U_k(F_k) = \sum_k U_k(F_k'), \quad F_k' = \omega F_k^{eq} + (1-\omega) F_k.$$

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]

Order tests

The test is done with the Burgers equation.

	Scheme 0		Scheme 1		Scheme 2	
Δx	L^2 error	order	L^2 error	order	L^2 error	order
2.000E-03	8.592E-05		3.370E-06		3.374E-06	
1.250E-03	3.358E-05	2.00	1.552E-06	1.65	1.551E-06	1.65
7.813E-04	1.404E-05	1.86	1.742E-07	4.65	1.742E-07	4.65
4.883E-04	5.494E-05	2.00	3.365E-08	3.50	3.365E-08	3.50
3.053E-04	2.160E-06	1.99	5.184E-09	3.98	5.184E-09	3.98

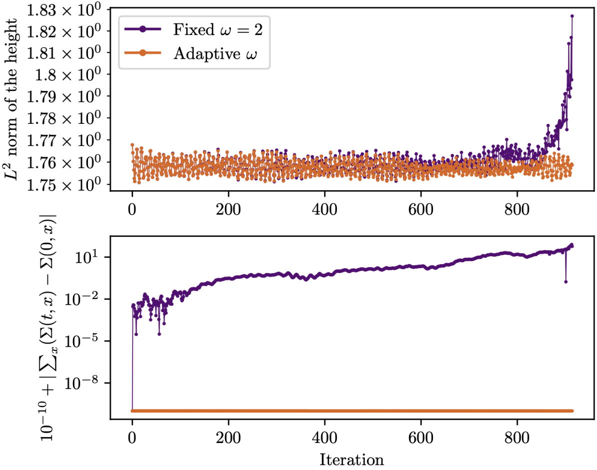
Scheme 0: second order LBM

Scheme 1: fourth-order time-symmetric LBM

Scheme 2: fourth-order with periodic projections

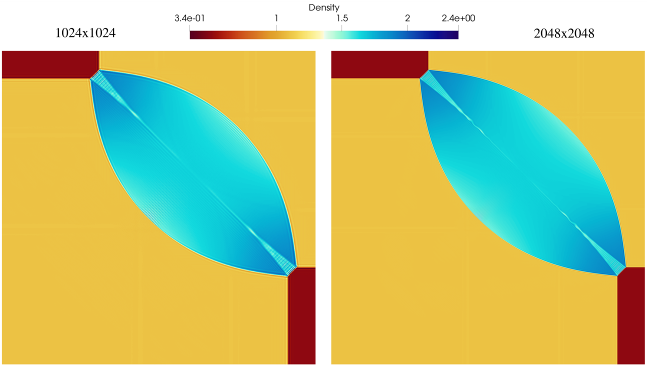
Stability tests

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

[Aregba-Driollet and Natalini(2000)] D. Aregba-Driollet and R. Natalini.
Discrete Kinetic Schemes for Multidimensional Systems of Conservation Laws.
SIAM J. Numer. Anal., 37(6):1973–2004, 2000.
doi: 10.1137/s0036142998343075.
URL https://doi.org/10.1137/s0036142998343075.

[Bellotti et al.(2024)Bellotti, Helluy, and Navoret] Thomas Bellotti, Philippe Helluy, and Laurent Navoret.
Fourth-order entropy-stable lattice Boltzmann schemes for hyperbolic systems.
working paper or preprint, March 2024.
URL https://hal.science/hal-04510582.

[Bouchut(1999)] F. Bouchut.
Construction of BGK Models with a Family of Kinetic Entropies for a Given System of Conservation Laws.
J. Stat. Phys., 95(1/2):113–170, 1999.
doi: 10.1023/a:1004525427365.
URL https://doi.org/10.1023%2Fa%3A1004525427365.

[Dellar(2013)] Paul J Dellar.
An interpretation and derivation of the lattice Boltzmann method using Strang splitting.
Computers & Mathematics with Applications, 65(2):129–141, 2013.

[Dubois(2008)] François Dubois.
Equivalent partial differential equations of a lattice Boltzmann scheme.
Computers & Mathematics with Applications, 55(7):1441–1449, 2008.

[Guillon et al.(2023)Guillon, Hélie, and Helluy] Kévin Guillon, Romane Hélie, and Philippe Helluy.
Stability analysis of the vectorial lattice-Boltzmann method.
working paper or preprint, 2023.
URL https://hal.science/hal-03986533.

Bibliography II

[Jin and Xin(1995)] Shi Jin and Zhouping Xin.
The relaxation schemes for systems of conservation laws in arbitrary space dimensions.
Communications on pure and applied mathematics, 48(3):235–276, 1995.

[McLachlan and Quispel(2002)] Robert I McLachlan and G Reinout W Quispel.
Splitting methods.
Acta Numerica, 11:341–434, 2002.