Stability analysis of an implicit lattice Boltzmann scheme

Philippe Helluy

Stability analysis of an implicit lattice Boltzmann scheme

Philippe Helluy

November 2016

IRMA, Université de Strasbourg and Inria Tonus. 7 rue Descartes, 67000 Strasbourg, France. helluy@unistra.fr

Abstract

We analyze the D1Q3 lattice kinetic model, which is the simplest kinetic model representing the isothermal Euler equations. We show that it is entropy unstable but that it can be made stable if the transport step is solved with an implicit numerical scheme.

1 Introduction

Lattice kinetic models are essential in computational fluid dynamics. They are the key ingredient of the Lattice Boltzmann Method (LBM). The idea is to construct a kinetic interpretation of a hyperbolic system of conservation laws with a minimal set of velocities. In this report we analyze the D1Q3 lattice kinetic model, which is the simplest kinetic model representing the isothermal Euler equations. We show that it is unstable but that it can be made stable if the transport step is solved with an implicit scheme. The unknown of the D1Q3 model is a three-dimensional distribution function $f(x,t) \in \mathbb{R}^3$, where $x \in \mathbb{R}$ and $t \in [0,T]$ are respectively the space and time variable. The distribution function satisfies transport equations with a BGK relaxation source term [1]

$$f_t^i + v_i f_x^i = \frac{1}{\varepsilon}(M(f)^i - f^i), \quad i = 1 \dots 3, \tag{1}$$

where we have noted partial derivatives with indices ($f_t = \partial_t f$ for instance). The kinetic velocity takes only three values

$$v = (-\lambda, 0, \lambda),$$

where λ is a positive real number. The fluid macroscopic variables are the density $\rho(x,t)$, the momentum $q(x,t)$ and the momentum flux $z(x,t)$. As usual the fluid velocity is defined by

$$u = q/\rho.$$

The macroscopic variables are recovered by computing discrete moments of f

$$\begin{pmatrix} \rho \\ q \\ z \end{pmatrix} = P \begin{pmatrix} f^1 \\ f^2 \\ f^3 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 1 & 1 \\ -\lambda & 0 & \lambda \\ \lambda^2 & 0 & \lambda^2 \end{pmatrix}.$$

The constant sound speed of the isothermal fluid is denoted by $c > 0$. The discrete Maxwellian state $M(f)$ is then given by

$$M(f) = \frac{1}{\lambda^2} \begin{pmatrix} \rho u(u-\lambda)/2 + c^2\rho/2 \\ \rho(\lambda^2 - u^2 - c^2) \\ \rho u(u+\lambda^2)/2 + c^2\rho/2 \end{pmatrix} \tag{2}$$

in such a way that

$$PM(f) = \begin{pmatrix} \rho \\ q \\ \rho u^2 + c^2\rho \end{pmatrix}.$$

Multiplying the kinetic equation (1) by P we obtain

$$\begin{aligned} \rho_t + q_x &= 0, \\ q_t + z_x &= 0, \\ z_t + \lambda^2 q_x &= \frac{1}{\varepsilon}(q^2/\rho + c^2\rho - z). \end{aligned} \tag{3}$$

When $\varepsilon \to 0$, then formally $f = M(f)$ and from (3) we see that ρ and u satisfy the isothermal Euler equations

$$\begin{aligned} \partial_t \rho + \partial_x(\rho u) &= 0, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + c^2\rho) &= 0. \end{aligned} \tag{4}$$

The model (1), (2) is thus a minimalistic abstract kinetic interpretation of the isothermal Euler equation. It is also denoted as the "D1Q3" model in the lattice-Boltzmann community [3]. It can be extended to higher dimensions. For instance, in two or three dimensions it becomes the D2Q9 or D3Q27 models.

2 Numerical method and asymptotic expansion

A traditional method for solving numerically (1) is the first order Lie splitting algorithm. For applying one time step of the splitting algorithm, we start from a state that is close to equilibrium: $f = M(f) + O(\varepsilon)$. We first apply the free transport equation for a duration of Δt

$$f_t + v \cdot f_x = 0.$$

Then in a second stage of the same duration Δt we apply the local BGK return to equilibrium

$$f_t = \frac{1}{\varepsilon}(M(f) - f).$$

In the case of the D1Q3 model, this approach can lead to instabilities that are sometimes observed in LBM simulations [2]. Therefore, we replace the exact transport step by a first order implicit solver in time. Assuming high precision of the solver in the x variable the effect of the implicit solver can be modeled by

$$\frac{f(x,t) - f(x, t-\Delta t)}{\Delta t} + v f_x(x,t) = 0. \tag{5}$$

By a Taylor expansion, we find the equivalent equation of the implicit solver (5)

$$f_t + v f_x - \frac{\Delta t}{2} v^2 f_{xx} = O(\Delta t^2). \tag{6}$$

In a second step, we solve the differential equation exactly

$$f_t = \frac{1}{\varepsilon}(M(f) - f) = \frac{M - I}{\varepsilon} f.$$

This is easy because during the relaxation step ρ, q, and thus $M(f)$, are constant.

In the following, ε is a small parameter, but we assume that the vector field M is restricted to a manifold of f's on which

$$\frac{M - I}{\varepsilon} f = O(1). \tag{7}$$

In the literature this hypothesis is often formulated by saying that f remains close to a Maxwellian state and that the initial data are "well-prepared". Hypothesis (7) is crucial because it will allow us to apply the Baker-Campbell-Hausdorf (BCH) formula with the good ordering for estimating the equivalent equation of the splitting algorithm. Let us also point out that we assume that (7) remains true even if $\varepsilon \sim \Delta t$ or $\varepsilon \sim \Delta t^2$ for instance. For a more precise analysis of this hypothesis, we refer to [4] (Section VI.3 pages 388–392).

In the Lie formalism, one time-step of the splitting scheme can be written

$$\varphi(\tau) = \exp(\tau \frac{M - I}{\varepsilon}) \exp(\tau(-v\partial_x + \frac{1}{2}\tau v^2 \partial_{xx})) + O(\tau^3).$$

Now we apply the BCH formula

$$\exp(A)\exp(B) = \exp(A + B + \frac{1}{2}[A, B] + \frac{1}{12}([A, [A, B]] + [B, [B, A]]) + \cdots).$$

We obtain

$$\varphi(\tau) = \exp(\tau L) + O(\tau^3),$$

with

$$L = -v\partial_x + \frac{1}{2}\tau v^2 \partial_{xx} + \frac{M - I}{\varepsilon} + \frac{1}{2}\tau \left[\frac{M - I}{\varepsilon}, -v\partial_x\right].$$

Therefore at second order in time, the equivalent equation of the scheme is

$$f_t + v f_x - \frac{\Delta t}{2} v^2 f_{xx} - \frac{1}{2}\Delta t \left[\frac{M - I}{\varepsilon}, -v\partial_x\right] f = \frac{M(f) - f}{\varepsilon}.$$

For expressing the Lie bracket in a more convenient way, we introduce the matrix

$$V = \begin{bmatrix} -\lambda & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \lambda \end{bmatrix}.$$

Then the Lie bracket becomes

$$\begin{aligned} [M - I, -v\partial_x] f &= -V\partial_x M(f) + M'(f) V \partial_x f \\ &= (M'V - VM')\partial_x f \end{aligned}$$

Now we go back to variables (ρ, q, z). After some computations, we find that

$$P\,[M - I, -v\partial_x]\,P^{-1} \begin{bmatrix} \rho \\ q \\ z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ -c^2 + u^2 & -2u & 1 \\ 0 & c^2 - \lambda^2 - u^2 & 2u \end{bmatrix} \partial_x \begin{bmatrix} \rho \\ q \\ z \end{bmatrix}.$$

We obtain the equivalent equations solved by the splitting algorithm at order 2 in Δt

$$\begin{aligned}
\rho_t + q_x - \frac{\Delta t}{2} z_{xx} &= 0, \\
q_t + z_x - \frac{\Delta t}{2}\lambda^2 q_{xx} &= \frac{\Delta t}{2\varepsilon}\left((u^2 - c^2)\rho_x - 2uq_x + z_x\right), \\
\partial_t z + \lambda^2 \partial_x q - \frac{\Delta t}{2}\lambda^2 z_{xx} &= \frac{1}{\varepsilon}(q^2/\rho + c^2\rho - z) + \frac{\Delta t}{2\varepsilon}\left((c^2 - \lambda^2 - u^2)q_x + 2uz_x\right).
\end{aligned} \tag{8}$$

On this equation we will now assume that $1 \gg \Delta t > \varepsilon$. We freeze Δt and perform a Chapman-Enskog expansion when $\varepsilon \to 0$. The second equation implies that when $\varepsilon \to 0$

$$z_x = (c^2 - u^2)\rho_x + 2uq_x = (q^2/\rho + c^2\rho)_x + O(\varepsilon)$$

and is thus redundant with

$$z = q^2/\rho + c^2\rho + O(\varepsilon).$$

The third equation in (8) gives

$$z = q^2/\rho + c^2\rho - \varepsilon\left(\partial_t z + \lambda^2\partial_x q\right) + \frac{\Delta t}{2}\left((c^2 - \lambda^2 - u^2)q_x + 2uz_x\right) + O(\varepsilon\Delta t).$$

We need to rewrite the factor in ε:

$$\partial_t z + \lambda^2 \partial_x q,$$

with only spatial derivatives. At leading order we have

$$\begin{aligned}
\partial_t z &= \partial_t\left(q^2/\rho + c^2\rho\right) + O(\varepsilon + \Delta t) \\
&= \frac{2q}{\rho}q_t - \frac{q^2}{\rho^2}\rho_t + c^2\rho_t + O(\varepsilon + \Delta t).
\end{aligned}$$

But $q_t = -z_x + O(\varepsilon + \Delta t)$ and $\rho_t = -q_x + O(\varepsilon + \Delta t)$ thus

$$z_t = -2uz_x + u^2 q_x - c^2 q_x + O(\varepsilon + \Delta t).$$

Then

$$z_t = -2u\left(2uq_x + (c^2 - u^2)\rho_x\right) + (u^2 - c^2)q_x + O(\varepsilon + \Delta t).$$

Finally

$$z_t + \lambda^2 q_x = \left(-3u^2 + \lambda^2 - c^2\right)q_x - 2u\left(c^2 - u^2\right)\rho_x + O(\varepsilon + \Delta t).$$

We then obtain the equivalent viscous equation of the splitting method

$$\begin{aligned}
\rho_t + (\rho u)_x &= \kappa\frac{\Delta t}{2}z_{xx}, \\
(\rho u)_t + \left(\rho u^2 + c^2\rho\right)_x &= \kappa\frac{\Delta t}{2}\lambda^2 q_{xx} + D_x,
\end{aligned}$$

with $\kappa = 1$ (effect of the implicit solver) or $\kappa = 0$ (exact transport solver) and

$$D = (\varepsilon + \frac{\Delta t}{2})\left(\left(\lambda^2 - c^2 - 3u^2\right)q_x + 2u\left(u^2 - c^2\right)\rho_x\right).$$

3 Stability analysis

Now we want to analyze the entropy stability of the second order term when $\varepsilon \to 0$. For this, we define

$$w = \begin{pmatrix} \rho \\ q \end{pmatrix}, \quad F(w) = \begin{pmatrix} q \\ \frac{q^2}{\rho} + c^2\rho \end{pmatrix}, \quad A(w) = \begin{pmatrix} \kappa(c^2 - u^2) & 2\kappa u \\ 2u\left(u^2 - c^2\right) & (1+\kappa)\lambda^2 - c^2 - 3u^2 \end{pmatrix},$$

and thus second order equivalent equations become

$$w_t + F(w)_x = \frac{\Delta t}{2}\left(A(w)w_x\right)_x \tag{9}$$

An entropy of the Euler equations is

$$S(w) = \frac{q^2}{2\rho} + c^2\rho\ln\rho.$$

We know that with this choice there exists an entropy flux $G(w)$ such that

$$S'F' = G'.$$

Multiplying (9) on the left by $S'(w)$, integrating by part in x and neglecting boundary terms, we obtain the entropy dissipation balance

$$\frac{d}{dt}\int_x S = -\frac{\Delta t}{2}\int_x w_x \cdot S''(w)A(w)w_x.$$

A sufficient condition for entropy dissipation is thus that $E(w) = S''(w)A(w)$ is a positive matrix. The D1Q3 model is generally used for subsonic flows. When $\kappa = 0$ (no numerical viscosity) $E(w)$ has always a negative eigenvalue and the scheme is thus unstable. The negative eigenvalue has a minimal modulus if $\lambda = \sqrt{3}c$ and is then of order $O(u^6)$. It justifies the fact that the scheme can, however, be applied in practice on relatively coarse meshes for low Mach number flows. When $\kappa \neq 0$ Taylors expansions in u show that

$$\begin{aligned} \rho^2\det(E(w)^T + E(w)) &= -4\,c^6 + 8\,\lambda^2 c^4 + O\left(u^2\right), \\ \rho\mathrm{Tr}(E(w)^T + E(w)) &= 2\,c^4 - 2\,c^2 + 4\,\lambda^2 + O(u^2). \end{aligned}$$

If λ is large enough, the scheme is thus stable for low Mach flows.

References

[1] Prabhu Lal Bhatnagar, Eugene P Gross, and Max Krook. A model for collision processes in gases. i. small amplitude processes in charged and neutral one-component systems. *Physical review*, 94(3):511, 1954.

[2] François Dubois. Stable lattice boltzmann schemes with a dual entropy approach for monodimensional nonlinear waves. *Computers & Mathematics with Applications*, 65(2):142–159, 2013.

[3] YH Qian, Dominique d'Humières, and Pierre Lallemand. Lattice bgk models for navier-stokes equation. *EPL (Europhysics Letters)*, 17(6):479, 1992.

[4] G Wanner and E Hairer. *Solving ordinary differential equations, stiff and differential-algebraic problems, second edition.*