Lattice and discrete Boltzmann equations for fully compressible flow

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Equilibria for the common two-dimensional, nine-velocity (D2Q9) lattice Boltzmann equation are not uniquely determined by the Navier–Stokes equations. An otherwise undetermined function must be chosen to suppress grid-scale instabilities. By contrast, the Navier–Stokes–Fourier equations with heat conduction determine unique equilibria for a one-dimensional, five-velocity (D1Q5) model on an integer lattice. Although these equilibria are subject to grid-scale instabilities under the usual lattice Boltzmann streaming and collision steps, the equivalent discrete Boltzmann equation is stable when discretized using conventional finite volume schemes. For flows with substantial shock waves, stability is confined to a window for the parameter controlling the mean free path. It is constrained between needing a large enough mean free path (large enough viscosity) to provide dissipation at shocks, and a small enough mean free path to ensure valid hydrodynamic behavior.

Keywords: lattice Boltzmann; discrete Boltzmann; compressible flow; shock waves

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I. INTRODUCTION

Methods based on the lattice Boltzmann equation (LBE) have become very popular for simulating incompressible fluids, for an overview see Chen & Doolen [1] or Succi [2]. The most common form of LBE simulates a compressible, isothermal fluid, and one chooses a ratio of fluid to sound speeds (Mach number) small enough to justify neglecting compressibility. The LBE is less well developed for simulating fully compressible flows with temperature variations, and possibly shock waves, or even just barotropic fluids with alternative equations of state like the shallow water equations.

Following the kinetic theory of gases, an LBE is an evolution equation for a distribution function $f_i(\mathbf{x},t)$ that specifies the number density of particles at a given location moving with a given velocity $\boldsymbol{\xi}_i$,

$$\partial_t f_i + \boldsymbol{\xi}_i \cdot \nabla f_i = -\frac{1}{\tau}(f_i - f_i^{(0)}). \tag{1}$$

Most current lattice Boltzmann equations use the Bhatnagar–Gross–Krook [3] collision operator on the right hand side of Eq (1). This relaxes the distribution function towards an explicitly specified equilibrium $f_i^{(0)}$ with a single timescale τ. By contrast, the Maxwell–Boltzmann equilibrium in continuum kinetic theory emerges from Boltzmann's binary collision operator as the distribution that extremises entropy while conserving mass, momentum, and energy. Determining the discrete equilibrium distribution is usually the most challenging part of constructing a viable LBE.

Macroscopic variables like fluid density ρ and momentum $\rho\mathbf{u}$, and their fluxes, are expressed as moments of the distribution function. From the first few moments of (1) we obtain

$$\partial_t\rho + \nabla\cdot(\rho\mathbf{u}) = 0, \quad \partial_t(\rho\mathbf{u}) + \nabla\cdot\mathbf{\Pi} = 0, \quad \rho = \sum_i f_i, \quad \rho\mathbf{u} = \sum_i \boldsymbol{\xi}_i f_i, \quad \mathbf{\Pi} = \sum_i \boldsymbol{\xi}_i\boldsymbol{\xi}_i f_i, \tag{2}$$

where the moments are expressed as sums rather than integrals because the velocities are discrete.

The Chapman–Enskog expansion seeks slowly varying solutions to Eq (1) such that the momentum flux $\mathbf{\Pi}$ and corresponding heat flux may be calculated without knowledge of higher moments. One way to derive the equilibria for an LBE is thus to ensure that every discrete moment of the equilibria that appears in the continuum equations via the Chapman–Enskog expansion coincides with the corresponding integral moment of the continuum Maxwell–Boltzmann distribution. In fact, He & Luo [4] showed that the most common equilibria for the two-dimensional, nine-velocity (D2Q9) lattice shown in Figure 1 may be derived using Gaussian quadrature to relate the discrete and integral moments.

However, Dellar [5] showed that Gaussian quadrature fails for general equations of state, and in particular for the shallow water equations. The resulting equilibria are unstable, but different and stable equilibria were found previously by Salmon [6]. The difficulty arises because the moments appearing in the Chapman–Enskog expansion do not determine the equilibria uniquely. By deriving a wave equation describing short-wave density fluctuations, Dellar [5] determined stable equilibria for any barotropic equation of state. The same situation arises when using a one-dimensional, five-velocity lattice (D1Q5) with a barotropic equation of state.

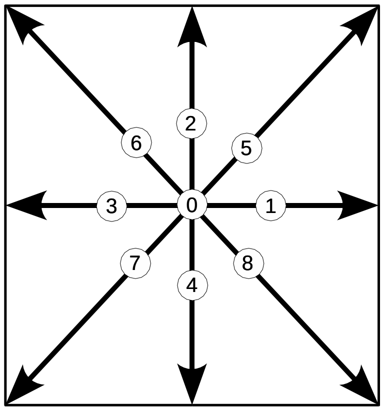
For fully compressible, varying temperature flows, the diffusive transport of heat provides an extra equation, so the D1Q5 equilibria are uniquely determined. These equilibria have not attracted much attention because they lead to grid-scale instabilities when implemented using the usual lattice Boltzmann discretization in space and time, under which Eq (1) is approximated by

$$\overline{f}_i(\mathbf{x}+\boldsymbol{\xi}_i\Delta t, t+\Delta t) - \overline{f}_i(\mathbf{x},t) = -\frac{\Delta t}{\tau+\Delta t/2}\left(\overline{f}_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right), \tag{3}$$

and the $\overline{f}_i$ are related to the f_i by

$$\overline{f}_i(\mathbf{x},t) = f_i(\mathbf{x},t) + \frac{\Delta t}{2\tau}\left(f_i(\mathbf{x},t) - f_i^{(0)}(\mathbf{x},t)\right). \tag{4}$$

FIG. 1: Arrangement of velocity vectors $\boldsymbol{\xi}_i$, where $i = 0, \ldots, 8$, for the two dimensional, nine velocity (D2Q9) lattice.



One may go from the partial differential equation Eq (3) to a lattice Boltzmann equation (1) by integrating along characteristics with the trapezium rule for a timestep Δt.

However, we find that these equilibria lead to stable simulations when discretized using conventional finite volume schemes. By contrast, the non-polynomial equilibria proposed by Renda *et al.* [7] and Ansumali *et al.* [8], produce solutions with noticeable artifacts (such as the compound waves found by Dellar [9]) due to the higher moments being incorrect. Moreover, the non-polynomial equilibria found by Ansumali *et al.* [8] by extremising a discrete entropy require a conventional finite volume discretization anyway, as their particle velocities are not integer multiples of each other. One might then just as well use the polynomial equilibria given below. They are also stable and do not yield unphysical artifacts.

II. BAROTROPIC FLOW WITH THE D1Q5 LATTICE

The most general equilibria yielding the one dimensional Navier–Stokes equations, with barotropic equation of state $p = P(\rho)$ for the pressure p, may be written as

$$f_i^{(0)} = w_i\big(\rho + \rho u \xi_i + \tfrac{1}{2}(P(\rho) - \rho + \rho u^2)(\xi_i^2 - 1) + \tfrac{1}{2}\rho u^3(\xi_i^3 - 3\xi_i) + g_i R^{(0)}\big), \quad (5)$$

where $R^{(0)}$ is an arbitrary function of ρ (at least) that is not determined by the Navier–Stokes equations. The five lattice velocities are $\xi_i = i$ for $i = -2, -1, 0, 1, 2$, with corresponding weights $w_0 = 1/2$, $w_{\pm 1} = 1/6$, and $w_{\pm 2} = 1/12$. The four lattice vectors 1, ξ_i, $\xi_i^2 - 1$ and $\xi_i^3 - 3\xi_i$ are all orthogonal with respect to these weights. They are completed by the vector $g_i = (1, -2, 1, -2, 1) = \xi_i^4 - 4\xi_i^2 + 1$ to form an orthogonal basis for $\mathbb{R}^5$.

For $p = \rho$ and $R^{(0)} = 0$, the equilibria in (5) coincide with those proposed by Qian & Zhou [10] for an isothermal equation of state with temperature $\theta = 1$. All choices of $R^{(0)}$ lead to the same continuum equations in the Chapman–Enskog expansion, but in general one must choose $R^{(0)} = (\rho - P(\rho))/2$ for stability against grid-scale oscillations, see Dellar [11]. The same situation holds for the D2Q9 lattice, see Dellar [5].

III. THERMAL FLOW WITH THE D1Q5 LATTICE

The continuum Maxwell–Boltzmann equilibrium in one spatial dimension is

$$f^{(0)} = \frac{\rho}{\sqrt{2\pi\theta}} \exp\left[-\frac{(\xi - u)^2}{2\theta}\right], \quad (6)$$

with the first five integral moments

$$\int f^{(0)} d\xi = \rho, \quad \int \xi f^{(0)} d\xi = \rho u, \quad \int \xi^2 f^{(0)} d\xi = \rho(\theta + u^2), \quad (7a)$$

$$\int \xi^3 f^{(0)} d\xi = \rho u(3\theta + u^2), \quad \int \xi^4 f^{(0)} d\xi = \rho(3\theta^2 + 6\theta u^2 + u^4). \quad (7b)$$

All five moments appear in the Chapman–Enskog expansion leading to the Navier–Stokes–Fourier equations describing gases with viscosity and thermal conduction. The last moment $\int \xi^4 f^{(0)} d\xi$ controls thermal diffusion. It does not appear in the barotropic Navier–Stokes equations, which is why $R^{(0)}$ was previously arbitrary.

Matching the five moments in Eq (7) defines a unique set of equilibria for a discrete Boltzmann equation using five particle velocities on an integer lattice. They may be written as

$$\begin{aligned} f_i^{(0)} = \rho w_i\Big(1 + u\xi_i \;&+\; \frac{1}{2}(\theta + u^2 - 1)(\xi_i^2 - 1) + \frac{1}{2}[u(3\theta + u^2) - 3u](\xi_i^3 - 3\xi_i) \\ &+\; \frac{1}{2}[3\theta^2 + 6\theta u^2 + u^4 - 4(\theta + u^2) + 1](\xi_i^4 - 4\xi_i^2 + 1)\Big), \end{aligned} \quad (8)$$

with the same weights w_i and lattice velocities $\xi_i = i$ as before.

No freedom is left to adjust the equilibria to suppress grid-scale instabilities, and the equilibria in Eq (8) are not useful in a conventional lattice Boltzmann method like Eq (3) because they are unstable. However, the instabilities disappear if we allow ourselves to use other spatial discretizations of Eq (1) instead.

Figure 2 shows a simulation of Sod's first shock tube using the equilibria from Eq (8) in a finite volume formulation of Eq (1) with Leonard's [12] third order upwind fluxes, and the second order accurate Runge–Kutta time integration described by Shu & Osher [13]. The grid had 8192 points, and the relaxation time was $\tau = 0.2$ in lattice units. The initial conditions correspond to a stationary gas with density and pressure given by

$$\rho = 1 \text{ and } p = 1 \text{ for } x < 0, \quad \rho = 0.125 \text{ and } p = 0.1 \text{ for } x > 0. \tag{9}$$

Leonard's [12] scheme gives extremely crisp shocks, at the price of some overshoot in neighbouring grid points unless the relaxation time τ is carefully tuned to supply adequate dissipation. The local Lax–Friedrichs or Rusanov fluxes, and their second order extension by Kurganov & Tadmor [14], may also be used. A small bump is also visible in the velocity, which is probably an artifact of smoothing these discontinuous initial conditions with a tanh profile over a few grid points. Both artifacts are far less prominent than in other schemes using non-polynomial equilibria.

For flows with substantial shock waves, like this example, stability is confined to a window in the relaxation time τ. The viscosity (proportional to τ) must be large enough to provide dissipation at shocks, but the mean free path (also proportional to τ) must be small enough to ensure hydrodynamic behavior. In other words, the Reynolds number Re and the Knudsen number Kn must both be sufficiently small, while subject to the constraint that $Kn = Ma/Re$ for fixed Mach number. For nearly-incompressible flows the Knudsen number may be made small at any desired Reynolds number by lowering the Mach number sufficiently.

For very large values of τ the solution becomes stable again, but does not describe hydrodynamics. The effect of collisions is so weak that the solution resembles free molecular flow. Figure 3 shows a typical example, with $\tau = 100$ in lattice units.

FIG. 2: Reproduction of Sod's first shock tube using a finite volume discretization of the discrete Boltzmann equation with $\tau = 0.2$. The Boltzmann solution has a slight overshoot at the shock, and a small bump in the velocity.

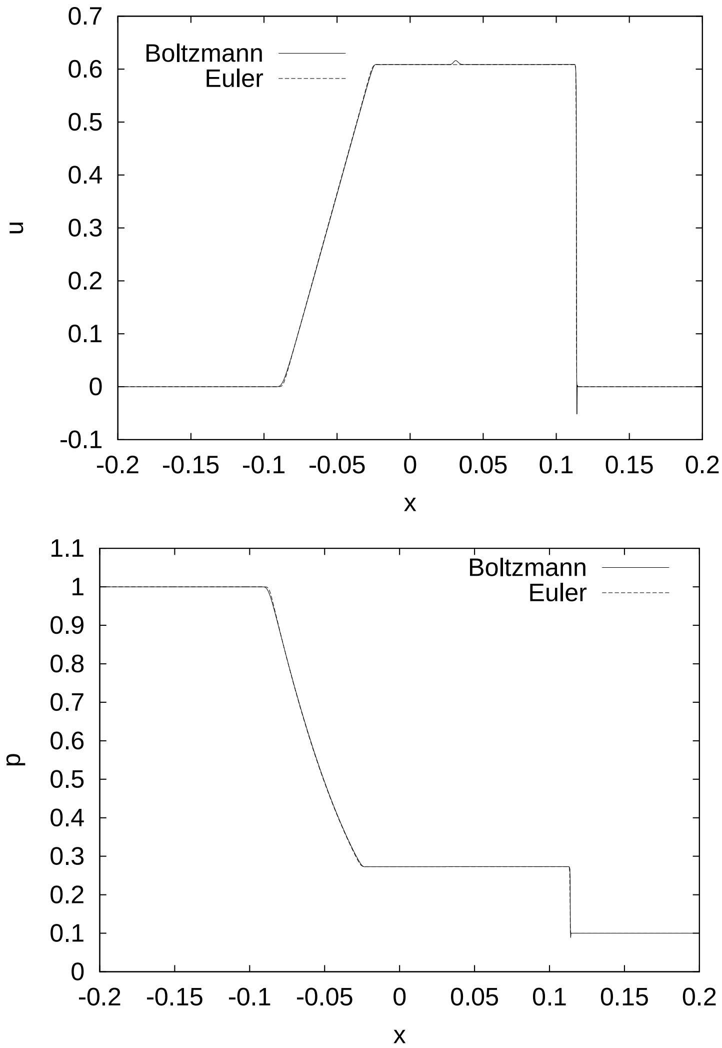
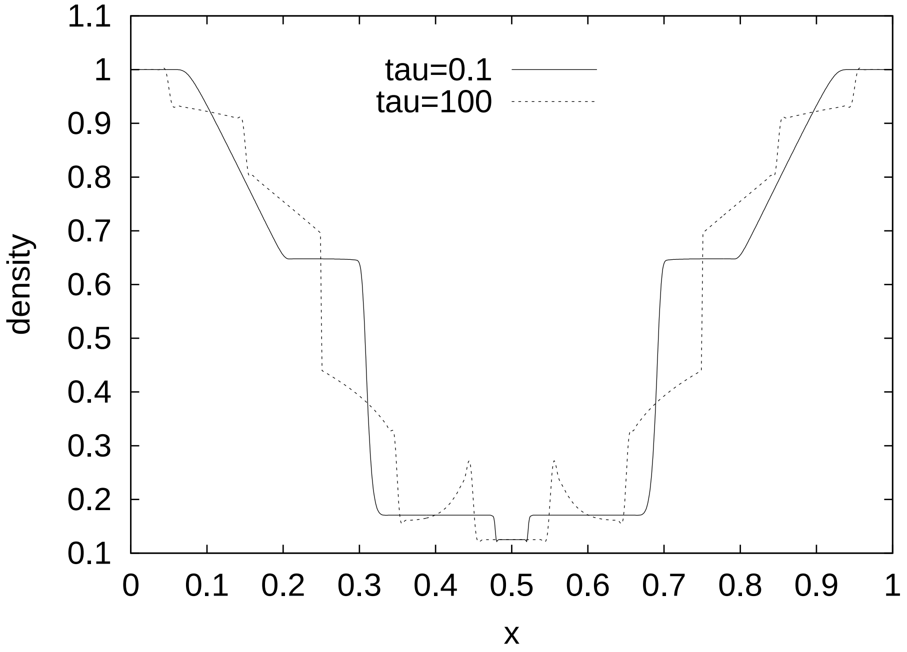


FIG. 3: Return to stability, but not correct hydrodynamics, for large values of τ. The behavior resembles free molecular flow, which is stable since distribution functions are purely advected.



IV. CONCLUSION

Unlike most lattice Boltzmann schemes for barotropic equations of state, the equilibria for a one-dimensional, five-velocity scheme simulating fully compressible flow with varying temperature are uniquely determined by the five moments necessary to recover the Navier–Stokes–Fourier equations. These unique equilibria are polynomials in the fluid velocity u. Although they lead to an unstable scheme using the standard lattice Boltzmann discretization, they may be used successfully with alternative finite volume discretizations of the discrete Boltzmann PDE to simulate flows with substantial shock waves. Any alternative equilibria will give unphysical artifacts, like compound waves or spikes, due to incorrect fluxes from the higher moments.

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