Entropic Lattice Boltzmann Models for Hydrodynamics in Three Dimensions

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Efficient, nonlinearly stable entropic lattice Boltzmann models for computational fluid dynamics are presented. A new method of fast evaluation of equilibria to machine precision is proposed. Analytical solution is found for the collision step which guarantees stability and thermodynamic consistency of the scheme. As an example, a novel 15-velocity lattice Boltzmann model is derived and validated with a simulation of a three-dimensional backward-facing step flow.

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In recent years, the lattice Boltzmann method (LBM) has become a mainstream tool in the computational approach to incompressible and weakly compressible flows. Applications of LBM range from hydrodynamics at large Reynolds numbers to flows at a micron scale, porous media, and multiphase flows [1]. LBM solves a fully discrete kinetic equation for populations $f_i(\boldsymbol{x}; t)$. Populations correspond to discrete velocities $\mathbf{c}_i$, $i = 1, \ldots, n_d$, which fit into a regular spatial lattice with the nodes $\boldsymbol{x}$. This enables a simple ''stream-along-links-and-equilibrate-at-nodes'' realization of the LBM algorithm.

Infamous limitation of the standard LBM is the inability to attain low viscosities because of numerical instabilities [1]. Hence, large Reynolds numbers in the standard LBM simulation can be achieved only by grid enlargement. Recent theoretical development of the entropic lattice Boltzmann method (ELBM) [2–7] alleviates this obstacle by restoring the second law of thermodynamics (Boltzmann's H theorem). This basic physical requirement renders the method nonlinearly stable numerically.

Entropic LBM in three dimensions is known for a highly symmetric lattice (discrete velocities are all possible tensor products of three one-dimensional velocity sets $\{-1, 0, 1\}$, the total number is 27). This model has been derived in various ways, including a variational method [3] and discretization of the continuous Boltzmann equation [7,8], and was recently extended to weakly compressible flow simulation [9]. Recently, the three-dimensional ELBM [7] was run on *Earth Simulator* and other massively parallel supercomputer facilities [10], and it was possible to attain extremely low viscosity in simulation of classical problems such as Taylor-Green and Kida vortex flows. This benchmark demonstrated maturity of the ELBM as a tool for turbulence simulations. However, a critical breakthrough in the efficiency of the lattice Boltzmann models is required.

In this Letter, the much needed breakthrough in the efficiency for ELBM is achieved. For the sake of concreteness, we consider a new entropic lattice Boltzmann model for a commonly used three-dimensional lattice with 15 velocities. We demonstrate that the fact the equilibrium is defined from the maximum entropy principle results in a method of *fast evaluation of equilibria to machine precision*. This method outperforms the traditional polynomial approximations used in LBM in terms of both efficiency and accuracy. Moreover, it does not scale with the number of discrete velocities, and therefore opens door for practicing LBM on large, highly isotropic velocity sets [7]. Finally, we derive analytical solution for the constraint on the relaxation step imposed by second law of thermodynamics. The new three-dimensional entropic lattice Boltzmann model derived herein enables highly efficient simulation of hydrodynamics.

Entropic LBM solves the kinetic equation [7],

$$f_i(\boldsymbol{x} + \mathbf{c}_i\delta t, t + \delta t) = f_i(\boldsymbol{x}, t) + \alpha\beta[f_i^{\mathrm{eq}}(\boldsymbol{x}, t) - f_i(\boldsymbol{x}, t)], \tag{1}$$

where

$$\beta = \frac{\delta t}{2\tau + \delta t}. \tag{2}$$

Here $\tau > 0$ is the relaxation time related to the kinematic viscosity, $\nu = \tau c_s^2$, where c_s is the speed of sound of the model, and δt is the discrete time step. In (1), one requires that the equilibrium populations, f_i^{eq}, minimize a convex entropy function H under constraints of local conservation of density and momentum.

Furthermore, in Eq. (1), $\alpha > 0$ is the nontrivial root of the entropy estimate,

$$H(f + \alpha(f^{\mathrm{eq}} - f)) = H(f). \tag{3}$$

Physically, the entropy estimate (3) defines the maximally possible change of populations in the relaxation step: the

entropy in the postrelaxation state, $f + \alpha(f^{\mathrm{eq}} - f)$, equals the entropy of the precollision state f. The needed amount of dissipation due to viscosity is brought into the kinetic equation (1) by the factor β (2). The entropy estimate (3) guarantees nonlinear stability of the scheme (1) since the total entropy, $H_{\mathrm{tot}} = \Sigma_x H(x)$, is a nonincreasing Lyapunov function of (1). When populations tend to the local equilibrium, then the solution of (3) converges to the equilibrium value $\alpha^{\mathrm{eq}} = 2$. If the value $\alpha = \alpha^{\mathrm{eq}}$ is used in (1), the standard LBM is recovered. The zero-viscosity limit corresponds to $\beta \to 1$. Efficient evaluation of α will be considered below.

Let us first consider the derivation of the local equilibrium $f_i^{\mathrm{eq}}(f)$, which depends on the populations f via locally conserved fields, density $\rho(f)$, and momentum $\rho \boldsymbol{u}(f)$ in such a way that

$$\rho = \sum_{i=1}^{n_d} f_i^{\mathrm{eq}}(\rho, \boldsymbol{u}), \qquad \rho \boldsymbol{u} = \sum_{i=1}^{n_d} \mathbf{c}_i f_i^{\mathrm{eq}}(\rho, \boldsymbol{u}). \tag{4}$$

Earlier derivations of the 27-velocity model have led to a Boltzmann entropy function [3,7]. Here, in order to derive H for the 15-velocity model, we begin with the Boltzmann ansatz for the entropy function,

$$H = \sum_{i=1}^{n_d} f_i \ln\left(\frac{f_i}{W_i}\right), \tag{5}$$

where the weights $W_i > 0$ are derived below. Equilibria f_i^{eq} are derived as the minimizer of H of the form (5) under constraints (4). The solution to this minimization problem can be written in the following product form:

$$f_i^{\mathrm{eq}} = W_i \chi \zeta_x^{cix} \zeta_y^{ciy} \zeta_z^{ciz}, \tag{6}$$

where Lagrange multipliers $\chi(\rho, \boldsymbol{u})$ and $\zeta_\alpha(\rho, \boldsymbol{u})$ are found upon substituting (6) into the constraints (4). The weights W_i are derived in such a way that the Navier-Stokes equation for low Mach number incompressible flow should be reconstructed by the kinetic equation (1). Namely, expanding the Lagrange multipliers into powers of the velocity components u_α around the zero-velocity solution $\chi(\rho, \mathbf{0}) = \rho$, $\zeta_\alpha(\rho, \mathbf{0}) = 1$, we find the weights W_i in such a way that the second-order approximation to the equilibrium satisfies the Maxwell-Boltzmann relation for the pressure tensor,

$$P_{\alpha\beta}^{\mathrm{eq}} = \sum_{i=1}^{n_d} f_i^{\mathrm{eq}}(\rho, \boldsymbol{u}) c_{i\alpha} c_{i\beta} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta, \tag{7}$$

where c_s is the speed of sound. For the 15-velocity lattice, the result reads

$$\begin{aligned}
c_{ix} &= \{0, 1, 0, 0, -1, 0, 0, 1, -1, 1, 1, -1, 1, -1, -1\},\\
c_{iy} &= \{0, 0, 1, 0, 0, -1, 0, 1, 1, -1, 1, -1, -1, 1, -1\},\\
c_{iz} &= \{0, 0, 0, 1, 0, 0, -1, 1, 1, 1, -1, 1, -1, -1, -1\},\\
W_i &= \frac{1}{72}\{16, 8, 8, 8, 8, 8, 8, 1, 1, 1, 1, 1, 1, 1, 1\},
\end{aligned} \tag{8}$$

while the speed of sound is $c_s = 1/\sqrt{3}$.

Functions χ and ζ_α in (6) are evaluated by perturbation around $\chi(\rho, \mathbf{0})$, $\zeta_\alpha(\rho, \mathbf{0})$, to order u^8 (we shall explain why below):

$$\begin{aligned}
\chi &= \rho\left(1 - \frac{3u^2}{2} + \frac{9u^4}{8} + \chi^{(6)} + \chi^{(8)}\right),\\
\chi^{(6)} &= \frac{27}{16}[-u^6 + 2(u_y^2 + u_z^2)(u^2 u_x^2 + u_y^2 u_z^2) + 20 u_x^2 u_y^2 u_z^2],\\
\chi^{(8)} &= \frac{81}{128} u^8 + \frac{81}{32}[u_x^8 + u_y^8 + u_z^8 - 36 u_x^2 u_y^2 u_z^2 u^2\\
&\quad - u_x^4 u_y^4 - u_y^4 u_z^4 - u_x^4 u_z^4];
\end{aligned} \tag{9}$$

$$\begin{aligned}
\zeta_\alpha &= 1 + 3u_\alpha + \frac{9{u_\alpha}^2}{2} + \frac{9{u_\alpha}^3}{2} + \frac{27{u_\alpha}^4}{8}\\
&\quad + \zeta_\alpha^{(5)} + \zeta_\alpha^{(6)} + \zeta_\alpha^{(7)} + \zeta_\alpha^{(8)},\\
\zeta_x^{(5)} &= \frac{27}{8}[u_x^5 - 4u_x u_y^2 u_z^2], \qquad \zeta_x^{(6)} = \frac{81}{16}[u_x^6 - 8u_x^2 u_y^2 u_z^2],\\
\zeta_x^{(7)} &= \frac{81}{16}[u_x^7 - 10 u_x^3 u_y^2 u_z^2 + 2u_x u_y^2 u_z^2 u^2],\\
\zeta_x^{(8)} &= \frac{243}{128}[u_x^8 + 16 u_x^2 u_y^2 u_z^2 (u_y^2 + u_z^2)],
\end{aligned} \tag{10}$$

where α can take the value x, y, or z. Corresponding expressions for $\zeta_y^{(i)}$ and $\zeta_z^{(i)}$ for $i = 5, 6, 7, 8$ are obtained by a cyclic permutation of x, y, and z.

Equation (6) together with Eqs. (9) and (10) give us the (eighth-order) product-form approximation to the equilibrium. Note that, when rational function (6) is further expanded to order u^8, one derives a polynomial approximation, $f_{i(n)}^{\mathrm{eq}}$, $n = 8$ in our case. Per our construction, polynomial approximations verify conservation laws (4) exactly. In particular, the second-order polynomial, $f_{i(2)}^{\mathrm{eq}}$, coincides with the equilibrium of the lattice Boltzmann model [11] and is sufficient to theoretically verify that the Navier-Stokes equations, with the kinematic viscosity $\nu = \tau c_s^2$, where $c_s = 1/\sqrt{3}$ is the speed of sound, are recovered in the hydrodynamic limit of the kinetic equation (1) when u is small enough. However, the use of $f_{i(2)}^{\mathrm{eq}}$ in simulations accumulates errors of order u^3, and it is quite important that one uses at least the fourth-order polynomials $f_{i(4)}^{\mathrm{eq}}$ in order to override this error. However, higher-order polynomials (although derived quite easily) come with an amplified computational cost.

The way out of this bottleneck is to use the product form (6) itself to evaluate the equilibria in a fast way (note that all $c_{i\alpha}$ are either 0 or 1, or -1). As a simple explanation, we remind that computation of $a^2 + 2ab + b^2$ requires six operations, while evaluation of the same expression as $(a + b)^2$ has just two. Evaluation of equilibria in the product form directly is thus overwhelmingly more efficient than evaluation of velocity polynomials.

Now, if the magnitude of the velocity is of the order $u \sim 10^{-2}$ (typical value used in accurate lattice Boltzmann simulations), then the difference between the eighth-order

product form (6) and the eighth-order polynomial $f^{\mathrm{eq}}_{i(8)}$ is less than 10^{-16}. Thus, for low Mach number flows, the product form (6) itself *verifies conservation laws to machine precision* (in double-precision arithmetics). In other words, although the approximate product-form equilibrium does not satisfy conservation laws (4) exactly, the residual is easily pushed to order u^9 which is *beyond* machine precision. If required, evaluating even higher-order terms in Eqs. (9) and (10) goes at only insignificant computational overhead, whereas evaluation of polynomial approximations of the same order becomes infeasible (see Table I).

In order to verify accuracy and efficiency of the product-form method, we simulate Couette flow using various strategies of computing equilibria, and with the standard lattice Boltzmann discretization [that is, setting $\alpha = 2$ in (1)]. In Fig. 1, the eighth-order product-form evaluation of (6) is compared to the fourth-order polynomial $f^{\mathrm{eq}}_{i(4)}$. Both the results match *exactly*. As indicated in Table I, the computational cost associated with the eighth-order product form is *less than half* of the computational cost of the fourth-order polynomial $f^{\mathrm{eq}}_{i(4)}$. Thus, the product-form evaluation of the equilibria outperforms polynomial approximations (or even closed form equilibria, if they are available, as in the case of the 27-velocity model [7]).

Note that the product form follows immediately from the fact that the equilibrium was defined as the minimum of the entropy function. Moreover, the computational demand does not scale with the number of discrete velocities (since the number of Lagrange multipliers, that is, the number of conservation laws, does not depend on the number of discrete velocities). This is again at striking variance with the polynomial approximations (see Table I), and can prove to be a turning point in constructing highly isotropic lattice Boltzmann models on large velocity sets. Results for the 64-velocity model [7] will be reported elsewhere.

Finally, let us consider the nonlinear stability, viz., the entropic time stepping process (3). In the previous approaches, Eq. (3) had to be solved for α, numerically at each lattice site. In order to minimize this computational effort, we remark that in most of the simulation domain, α is typically close to its local equilibrium value $\alpha^{\mathrm{eq}} = 2$. In these cases, the solution to Eq. (3) is readily obtained analytically. Namely, by expanding logarithms in the Eq. (3) in powers of $(f_i^{\mathrm{eq}} - f_i)/f_i$, it is easy to obtain the asymptotic expansion for the solution α, which we write here to third order:

$$\alpha = 2 - \frac{4a_2}{a_1} + \frac{16a_2^2}{a_1^2} - \frac{8a_3}{a_1} + \frac{80a_2a_3}{a_1^2} - \frac{80a_2^3}{a_1^3} - \frac{16a_4}{a_1}. \tag{11}$$

Coefficients a_n are as follows:

$$a_n = \frac{(-1)^{n-1}}{n(n+1)} \sum_{i=1}^{n_d} \frac{(f_i^{\mathrm{eq}} - f_i)^{n+1}}{f_i^n}, \qquad n \geq 1. \tag{12}$$

Formula (11) can be appreciated as a refinement of the equilibrium value $\alpha^{\mathrm{eq}} = 2$, to which (11) converges as $f \to f^{\mathrm{eq}}$. Application of (11) assumes setting a tolerance value for the deviation $|(f_i^{\mathrm{eq}} - f_i)/f_i|$ (typically, 10^{-2}). If the deviation is within the tolerance, the analytical formula (11) is applied, and for the remaining lattice sites, Newton-Raphson iterations are used to evaluate (3). In practice, the analytical expression (11) can be applicable at some 90% of grid points; thus, the nonlinear stability is achieved at virtually no computational overhead.

Simulation of the three-dimensional backwards-facing step flow was used to validate the new model. Geometry of the setup corresponds to the experiment of Armaly *et al.* [12]. A grid resolution of the 11 lattice points for the step height S was used, resulting in about 1.5×10^6 grid points for the simulations. The inflow was a fully developed velocity profile of a duct flow (simulated separately). The outflow boundary conditions of Ref. [13] were used. All simulations were done at a single-processor facility, a single run time ranged between one to several hours de-

TABLE I. Estimated operation count and accuracy of evaluation of equilibria for various discrete velocity sets.

Lattice	Accuracy	Operations
15 (3D)	u^4 (polynomial)	330
	u^8 (present)	120
27 (3D)	exact [7]	320
	u^8 (present)	160
16 (2D)	u^8 (polynomial) [7]	1000
	u^8 (present)	260
64 (3D)	u^5 (polynomial)	5000
	u^8 (present)	510

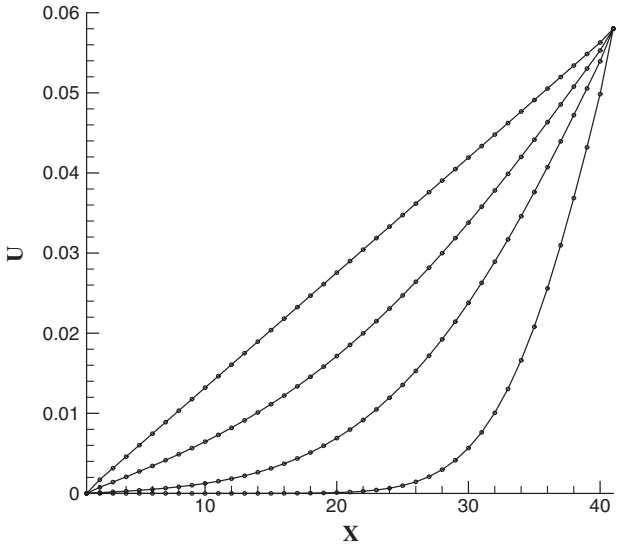

FIG. 1. Development of the velocity profile in Couette flow. Symbols: Fourth-order polynomial approximation. Lines: Eighth-order product-form method.

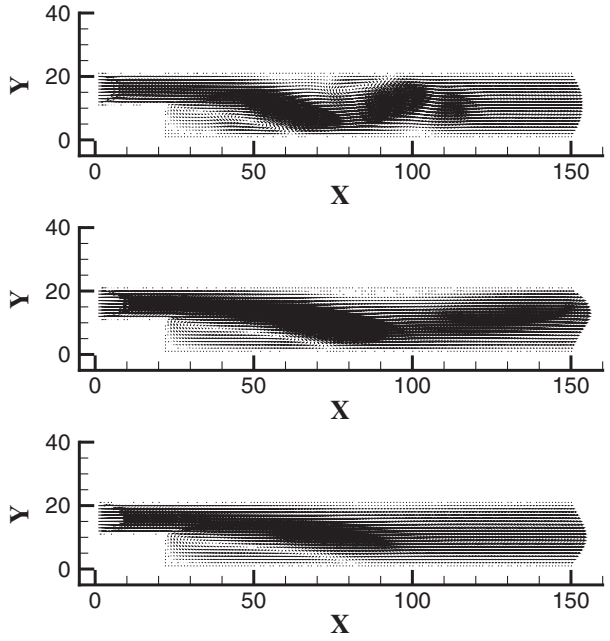

FIG. 2. Snapshots of the velocity field on the midplane at Re = 270 at 9×10^3, 18×10^3, and 40×10^3 time steps in lattice units (from top to bottom).

pending on the Reynolds number, $\mathrm{Re} = (2US)/\nu$, where U is cross-section averaged inlet velocity. The range of Reynolds number covered in our simulation was $100 < \mathrm{Re} < 392$. In Fig. 2, snapshots of the velocity on the midplane at Re = 270 are shown. In Fig. 3, the primary flow reattachment length is compared with simulations of the Navier-Stokes equations by various numerical techniques

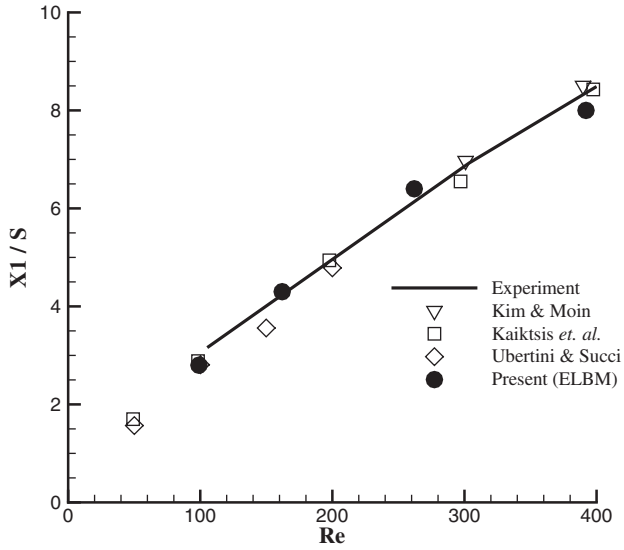

FIG. 3. Primary reattachment length X_1 normalized by the step height S. Comparison of the present simulation with the experiment [12] and reference simulation data [14–16].

[14,15], with the recent two-dimensional lattice Boltzmann simulation on a nonuniform grid [16], as well as with the experimental data of Armaly *et al.* [12]. The results were found to be in excellent agreement with each other.

In conclusion, we have derived a highly efficient, nonlinearly stable lattice Boltzmann model for simulations of three-dimensional incompressible flows. The scheme is easy to implement—the formulas presented above are sufficient. The method of fast evaluation of equilibrium to machine precision and the analytical solution for the entropy estimate open a new perspective on the minimal kinetic models: One is no longer restricted by computational efficiency, and can switch from models on long-known lattices with low symmetry to large discrete velocities sets with higher symmetry.

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