Consistent Lattice Boltzmann Method

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Lack of energy conservation in lattice Boltzmann models leads to unrealistically high values of the bulk viscosity. For this reason, the lattice Boltzmann method remains a computational tool rather than a model of a fluid. A novel lattice Boltzmann model with energy conservation is derived from Boltzmann's kinetic theory. Simulations demonstrate that the new lattice Boltzmann model is the valid approximation of the Boltzmann equation for weakly compressible flows and microflows.

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The overwhelming majority of fluid flows of physical and engineering interest are slow; i.e., characteristic flow speed u is small compared to the speed of sound c_s. This is quantified by the Mach number, $\mathrm{Ma} \sim u/c_s$, which typically varies from 10^{-3}–10^{-2} in hydrodynamic flows (turbines, reactors, etc.) to 10^{-4} in flows at a micrometer scale. The simplest characterization of the degree of molecularity is then the Knudsen number $\mathrm{Kn} \sim \lambda/H$, the ratio of the mean free path λ, and the characteristic scale H of variation of hydrodynamic fields (density, momentum, and energy). When $\mathrm{Kn} \lesssim 10^{-3}$, one considers the hydrodynamic limit where molecularity reduces to a set of transport coefficients (viscosity, thermal conductivity, etc.). If, in addition, the Mach number is also small, one obtains the incompressible hydrodynamics with the ordering $\mathrm{Kn} \ll \mathrm{Ma} \ll 1$, and the flow can be characterized solely by the ratio $\mathrm{Re} \sim \mathrm{Ma}/\mathrm{Kn}$ (one of the definitions of the Reynolds number).

Computational fluid dynamics becomes increasingly more interested in the domain where the Mach number remains small but the Knudsen number increases, and thus incompressibility becomes gradually lost. Because of its relevance to the engineering of microelectromechanical systems, the branch of computational fluid dynamics focused on microscale phenomena is often called "microfluidics" [1]. Flows in microdevices are highly subsonic (with characteristic flow velocities about 0.2 m/s, corresponding to $\mathrm{Ma} \sim 10^{-4}$), while the Knudsen number varies from $\mathrm{Kn} \sim 10^{-2}$ (so-called slip-flow regime) to $\mathrm{Kn} \sim 0.1$ (moderately rarefied gas flows) [1]. There is much need for computational models in the domain of slow flows. Indeed, such methods as molecular dynamics or direct simulation Monte Carlo are inefficient for slow flows at small Knudsen numbers [2].

In recent years, the lattice Boltzmann method has drawn considerable attention as a simulation method for flows at low Mach numbers. Especially popular are the isothermal lattice Boltzmann models (ILBM) without energy conservation [3]. In view of the impressive number of simulations including turbulent flows, ILBM can be regarded as the established method for hydrodynamic simulations. Owing to their outstanding computational features and established relations to the continuous kinetic theory [4–6], there is increasing interest in applying lattice Boltzmann models also to microflow simulation [1,7–10]. The hydrodynamic (locally conserved) fields in the ILBM are the density ρ and the momentum density $\boldsymbol{j}$, whereas the conservation of the energy is not addressed. All ILBM models have one point in common: The lack of energy conservation inevitably leads to a bulk viscosity. Indeed, the nonequilibrium part of the stress tensor in ILBM reads

$$P^{\mathrm{neq}}_{\alpha\beta} \sim \mathrm{Kn}\left[\partial_\alpha\left(\frac{j_\beta}{\rho}\right) + \partial_\beta\left(\frac{j_\alpha}{\rho}\right)\right]. \tag{1}$$

This tensor is not traceless, $P^{\mathrm{neq}}_{\alpha\alpha} \sim 2\mathrm{Kn}\partial_\alpha(j_\alpha/\rho)$, which immediately leads to the bulk viscosity terms in the equation for the momentum density. We recall that the physical bulk viscosity in hydrodynamic models is related to a redistribution of the energy among the translational and internal degrees of freedom of molecules rather than to any nonconservation of the energy. The physical bulk viscosity of fluids is typically much smaller than the shear viscosity. Thus, from the physical standpoint, the bulk viscosity of the ILBM is just spurious because its magnitude is of the order of the shear viscosity. Certainly, the presence of the bulk viscosity, spurious or not, by no means precludes the limit of incompressible hydrodynamics because, loosely speaking, the divergence of the velocity field $\boldsymbol{u} = \boldsymbol{j}/\rho$ vanishes in that limit [11]. Thus, ILBM is a valid model for the incompressible hydrodynamics. However, the spurious bulk viscosity of ILBM becomes a severe drawback when such models are applied to weakly compressible or microflow simulations.

The best way to illustrate this problem is to consider a representative example. Plane Poiseuille flow is one of the most studied benchmarks on gas dynamics. The gas moves between two parallel plates driven by a fixed pressure difference between the inlet and outlet. It is known from the classical kinetic theory [12] that the flow rate Q has the following asymptotic at low and high Knudsen numbers:

$$Q_0 = (6\mathrm{Kn})^{-1} + s + (2s^2 - 1)\mathrm{Kn}, \qquad \mathrm{Kn} \ll 1,$$
$$Q_\infty \sim (1/\sqrt{\pi})\ln(\mathrm{Kn}) + O(1), \qquad \mathrm{Kn} \to \infty,$$

with $s = 1.015$. These two asymptotic limits ensure that the flow rate has a minimum at some finite Kn (the Knudsen minimum [12]). While a qualitative agreement of the ILBM simulations with the continuous-velocity kinetic theory was found at all Knudsen numbers [9,10], the quantitative agreement is poor beyond the slip-flow regime at $\mathrm{Kn} > 10^{-2}$. It was found that the ILBM systematically overpredicts the flow rate at small Knudsen numbers. This is the effect of the bulk viscosity which can be qualitatively explained as follows: At low Knudsen numbers the behavior is still dominated by particle's collisions in the bulk; therefore, the steady state is reached upon a balance between the frictional force $\sim \mathrm{Kn}\partial_\beta P^{\mathrm{neq}}_{\alpha\beta}$ and the forcing due to the constant pressure gap between the inlet and the outlet. Thus, if there is additional contribution of the bulk viscosity (more friction), this balance at the same Kn shifts to a higher velocity at the steady state, and results in the overprediction of the flow rate.

In this Letter we introduce new lattice Boltzmann models with the energy conservation for weakly compressible flows. These models are derived from the continuous kinetic theory and are free from the drawbacks of the ILBM, and at the same time they retain in full the outstanding computational efficiency of the latter.

The starting point of our derivation is the grand canonic potential of the Boltzmann kinetic theory [12],

$$H = \int F \ln F d\mathbf{v} + \mu \int F d\mathbf{v} + \zeta_\alpha \int F v_\alpha d\mathbf{v} + \gamma \int F v^2 d\mathbf{v}, \tag{2}$$

where $F(\boldsymbol{x}, \mathbf{v})$ is the one-particle distribution function, and μ, ζ_α, and γ are Lagrange multipliers corresponding to density, momentum, and energy, respectively. The $D+2$-parametric family of functionals (2), where D is the dimension of the velocity space, describes the equilibrium states as its minima, $\delta H = 0$, and it also defines the locally conserved fields (density ρ, momentum $\boldsymbol{j}$, and energy e),

$$\frac{\partial H}{\partial \mu} = \rho, \qquad \frac{\partial H}{\partial \zeta_\alpha} = j_\alpha, \qquad \frac{\partial H}{\partial \gamma} = e. \tag{3}$$

In order to derive the discrete-velocity kinetic theory, functional (2) is evaluated with the D-dimensional Gauss-Hermite quadrature, with the Gaussian weight $W = (2\pi\theta_0)^{-D/2}\exp[-v^2/(2\theta_0)]$, where $\theta_0 = (k_B T_0/m)$ is the reduced uniform reference temperature. Quadrature evaluation of an integral replaces it by a sum, $\int W(\mathbf{v})G(\mathbf{v})d\mathbf{v} \approx \sum_{i=1}^{n_d} W_i G(\mathbf{v}_i)$, where $\mathbf{v}_i$, $i = 1, \ldots, n_d$, are the nodes of the quadrature, and W_i are corresponding weights. In our case, the nodes of the quadrature (discrete velocities) are at the zeroes of Hermite polynomials. For concreteness, we shall consider the third-order Hermite polynomial. Then $n_d = 3^D$, and the discrete velocities and weights are constructed as follows: For $D = 1$, the three roots and corresponding weights are $(-\sqrt{3\theta_0}, 0, \sqrt{3\theta_0})$ and $(1/6, 2/3, 1/6)$; for $D > 1$, the roots are all possible tensor products of the roots in $D = 1$, and the weights are corresponding products of one-dimensional weights. We shall consider $D = 3$ below, that is, $n_d = 27$ (same considerations apply to any quadrature, in particular, to the popular 9-velocity model for $D = 2$). As is well known, the third-order quadrature has the unique feature that its nodes form a face-centered cubic lattice, which is the crucial feature to the further lattice Boltzmann discretization in space and time. Introducing the populations, $f_i = W_i(2\pi\theta_0)^{3/2}\exp[v_i^2/(2\theta_0)]F(\boldsymbol{x}, \mathbf{v}_i)$, and using the reduced discrete velocities, $\boldsymbol{c}_i = \mathbf{v}_i/\sqrt{3\theta_0}$, we write the quadrature for (2) as

$$H = \sum_{i=1}^{27}\left\{f_i \ln\left(\frac{f_i}{W_i}\right) + \mu f_i + \zeta_\alpha f_i c_i + \gamma f_i c_i^2\right\}. \tag{4}$$

Differentiation of (4) with respect to Lagrange multipliers implies the locally conserved fields in the discrete case,

$$\sum_{i=1}^{27}\{1, c_{i\alpha}, c_i^2\}f_i = \{\rho, j_\alpha, 3p + \rho^{-1}j^2\}. \tag{5}$$

The equilibria f_i^{eq} are now found as minima of H (4). From the extremum condition, $\delta H = 0$, it follows that

$$f_i^{\mathrm{eq}} = W_i \exp\{-\mu - \zeta_\alpha c_{i\alpha} - \gamma c_i^2\}. \tag{6}$$

In order to express the Lagrange multipliers in (6) in terms of hydrodynamic fields (5), we substitute (6) into (5) and derive the functions $\mu(\rho, \boldsymbol{j}, p)$, $\zeta_\alpha(\rho, \boldsymbol{j}, p)$, and $\gamma(\rho, \boldsymbol{j}, p)$ by perturbation for small momentum, owing to the fact that $\zeta_\alpha(\rho, \mathbf{0}, p) = 0$, and that the zero-momentum functions $\mu(\rho, \mathbf{0}, p)$ and $\gamma(\rho, \mathbf{0}, p)$ can be found in a closed form. Computation is quite straightforward, and we write here the final result to second order in the momentum:

$$f_i^{\mathrm{eq}}(\rho, \boldsymbol{j}, p) = \rho\left(1 - \frac{p}{\rho}\right)^3\left(\frac{\frac{p}{\rho}}{2(1-\frac{p}{\rho})}\right)^{c_i^2}\left[1 + \frac{c_{i\alpha}j_\alpha}{p} + \frac{j_\alpha j_\beta}{2p^2} \times \left(c_{i\alpha}c_{i\beta} - \frac{6\frac{p^2}{\rho^2} + c_i^2(1 - 3\frac{p}{\rho})}{3(1-\frac{p}{\rho})}\delta_{\alpha\beta}\right)\right]. \tag{7}$$

The prefactor in this formula has the following limit when $(p/\rho) \to (1/3)$:

$$\lim_{(p/\rho)\to(1/3)}\left(1 - \frac{p}{\rho}\right)^3\left(\frac{\frac{p}{\rho}}{2(1-\frac{p}{\rho})}\right)^{c_i^2} = W_i. \tag{8}$$

The implication of (8) will be important below when discussing the relation of the present model to the ILBM.

We now proceed with the evaluation of the stress tensor $P^{\mathrm{eq}}_{\alpha\beta}(\rho, \boldsymbol{j}, p)$ and of the energy flux $q^{\mathrm{eq}}_{\alpha}(\rho, \boldsymbol{j}, p)$ at equilibrium. The important observation to be made here is that if the pressure to density ratio satisfies the condition $(p/\rho) = (1/3)$, then $P^{\mathrm{eq}}_{\alpha\beta}$ and q^{eq}_{α} satisfy the corresponding relations pertinent to the continuous-velocity Maxwell distribution. In dimensional units, the condition just mentioned reads $p = (k_B T_0 \rho)/m$; that is, it corresponds to the ideal gas equation of state at the reference temperature of the Gaussian weight. Moreover, if we allow small variations of the pressure around the point $p/\rho = 1/3$ [weakly compressible flows, $|(p/\rho) - (1/3)| \lesssim \mathrm{Ma}^2$], then Maxwell's form of $P^{\mathrm{eq}}_{\alpha\beta}$ and q^{eq}_{α} persists:

$$P^{\mathrm{eq}}_{\alpha\beta} = \sum_{i=1}^{27} f_i^{\mathrm{eq}} c_{i\alpha} c_{i\beta} = p\delta_{\alpha\beta} + \frac{j_\alpha j_\beta}{\rho}, \tag{9}$$

$$q^{\mathrm{eq}}_{\alpha} = \sum_{i=1}^{27} f_i^{\mathrm{eq}} c_{i\alpha} c_i^2 = 5\frac{p}{\rho} j_\alpha. \tag{10}$$

With the equilibrium (7), we write up the simplest kinetic equation [the Bhatnagar-Gross-Krook (BGK) model],

$$\partial_t f_i + c_{i\alpha}\partial_\alpha f_i = -\frac{1}{\tau}[f_i - f_i^{\mathrm{eq}}(\rho, \boldsymbol{j}, p)], \tag{11}$$

where $\tau > 0$ is the relaxation time. In order to find out the hydrodynamic limit of the model, we perform the Chapman-Enskog analysis at low Mach numbers. In so doing, we neglect all terms in j_α of the order of three and higher, and we end up with the following nonequilibrium expressions for the stress and the heat flux:

$$P^{\mathrm{neq}}_{\alpha\beta} = -\tau p\left[\partial_\alpha\left(\frac{j_\beta}{\rho}\right) + \partial_\beta\left(\frac{j_\alpha}{\rho}\right) - \frac{2}{3}\delta_{\alpha\beta}\partial_\gamma\left(\frac{j_\gamma}{\rho}\right)\right], \tag{12}$$

$$q^{\mathrm{neq}}_{\alpha} = -2\tau p\partial_\alpha\left(\frac{p}{\rho}\right). \tag{13}$$

The most important achievement is that now the nonequilibrium (Newtonian) stress (12) is traceless, as pertinent to the classical case of Boltzmann's fluid considered herein. That is, by preserving the energy conservation in the derivation, we eliminated the spurious bulk viscosity of ILBM. The heat flux (13) obeys the Fourier law. It should be noted that the present model does not solve the problem of bulk viscosity and heat conductivity entirely, nor can it be applied to highly compressible flows (supersonic flows, for example). However, the domain of validity is wide enough to include such important flows as convection flows and microflows.

We have implemented the lattice Boltzmann space-time discretization of the kinetic Eq. (11) and redone the micro-Poiseuille flow simulation mentioned in the introduction.

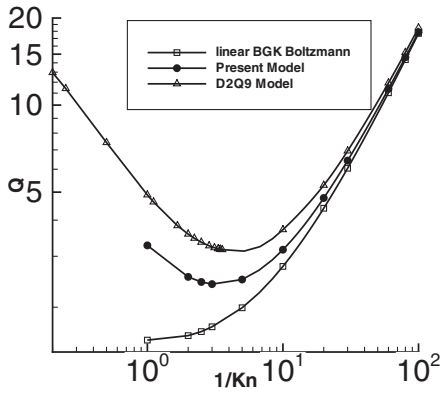

FIG. 1. Flow rate in the pressure driven Poiseuille flow as a function of inverse Knudsen number. Comparison of the present energy-conserving model with the isothermal lattice Boltzmann model [6] and the continuous linearized Boltzmann-BGK model [13].

The flow is driven by a constant pressure drop between the inlet and the outlet, and, as the kinetic theory suggests [12], the temperature variation is negligible. Results are presented in Fig. 1, where the present model is compared to the exact solution of the continuous linearized BGK model [13], and the $2DQ9$ isothermal lattice Boltzmann model with the spurious bulk viscosity [14]. It is clearly visible that the effect of the spurious bulk viscosity is eliminated at small Knudsen numbers, and that the quantitative agreement with the continuous BGK model extends up to $\mathrm{Kn} \sim 0.1$. For higher values of Knudsen numbers, the agreement remains qualitative. The reason is in the simplicity of the present model with only 27 velocities. Models with more velocities extend the domain further in Kn (see, e.g., [5,6]). However, from the standpoint of practical applications in microflow simulations, the domain $\mathrm{Kn} < 0.1$ is most relevant, and the present lattice Boltzmann model fits well into this domain.

In another simulation, we compared the present model with the steady-state temperature variation between two parallel walls kept at the temperatures T_{L} and T_{R} at a distance L. Analytical solution to the stationary continuous linearized BGK model reads [15] $T = [(T_{\mathrm{L}} - T_{\mathrm{R}})/(1 + 3.882\,34\mathrm{Kn})]x + [(T_{\mathrm{L}} + T_{\mathrm{R}})/2]$, where x is the dimensionless distance from the center of the channel. Diffusive wall boundary conditions [7] were applied, and a small temperature gap $T_{\mathrm{L}} - T_{\mathrm{R}}$ was considered (approximately 1% variations of the average temperature). Results are presented in Fig. 2. Quantitative agreement with the continuous kinetic theory up to $\mathrm{Kn} \sim 0.05$ is observed. We recall here that there is no adjustable slip coefficients, or other tunable parameters, in our simulation, and thus it is remarkable that the model is able to reproduce accurately the velocity and the thermal slip as known from the classical kinetic theory. This clearly demonstrates that the present lattice Boltzmann equation is a valid model of the Boltzmann equation for almost isothermal low Knudsen number flows.

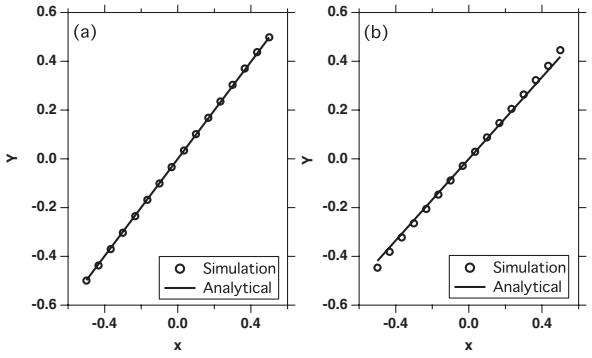

FIG. 2. Steady-state temperature variation between parallel walls. Reduced temperature $Y = (T - T_0)/(T_L - T_R)$ is shown as the function of the reduced distance x at (a) Kn = 0.001 and (b) Kn = 0.05. Symbols, simulation; line, analytical solution by Bassanini, Cercignani, and Pagani [15].

Finally, let us place our derivation with respect to previously reported lattice Boltzmann models on the same lattice. If we substitute $p = (1/3)\rho$ into the equilibrium function (7), and use the limit (8), then $f_i^{\mathrm{eq}}(\rho, \boldsymbol{j}, \rho/3)$ recovers the second-order polynomial equilibrium of the isothermal lattice Boltzmann method on the same lattice, and instead of the traceless stress tensor (12), we recover (1) with the bulk viscosity component. It needs to be stressed that the second-order polynomial in $\boldsymbol{j}$ (7) is an approximation to the positive-definite discrete-velocity equilibrium (6). Same as with the isothermal models, this second-order approximation simply happens to be good enough for stable computations at $\mathrm{Ma} < 0.1$. If we keep the relation $p = (1/3)\rho$ to all the orders in $\boldsymbol{j}$, we recover the exact positive-definite equilibrium of the isothermal 27-velocities entropic lattice Boltzmann model [6]:

$$f_i^{\mathrm{eq}}(\rho, \boldsymbol{j}, \rho/3) = \rho W_i \prod_{\alpha=1}^{3} (2 - \sqrt{1 + 3(j_\alpha/\rho)^2}) \times \left(\frac{2(j_\alpha/\rho) + \sqrt{1 + 3(j_\alpha/\rho)^2}}{1 - (j_\alpha/\rho)} \right)^{c_{i\alpha}}. \quad (14)$$

Our approach to the discretization of the velocity space differs from the earlier attempts [4,5]. While we use the same Gauss-Hermite quadrature, we apply it on the grand canonical potential (2) [that is, we evaluate the velocity integral (2) as pertinent to the meaning of a quadrature], and after that find the discrete-velocity equilibrium upon minimization of the discrete-velocity grand canonical potential (4). Instead, the authors of [4,5] evaluate the local Maxwellian (that is, they evaluate a *function*, not an integral) of continuous kinetic theory, $M(\rho, \boldsymbol{j}, T; \mathbf{v}) = \rho(2\pi k_B T/m)^{-D/2} \exp[-m(\mathbf{v} - \boldsymbol{u})^2/2k_B T]$, $\boldsymbol{u} = \boldsymbol{j}/\rho$, on the nodes of the quadrature. Certainly, just replacing $M(\rho, \boldsymbol{j}, T; \mathbf{v}) \to M_i(\rho, \boldsymbol{j}, T; \mathbf{v}_i)$ makes no sense because the conservation laws will be lost. However, it was noticed in [4] that if the second-order expansion of the Maxwellian is used instead, $M^{(2)} = \rho W(1 + a v_\alpha j_\alpha + b v_\alpha v_\beta j_\alpha j_\beta)$, the replacement, $M^{(2)} \to \rho W_i(1 + a v_{i\alpha} j_\alpha + b v_{i\alpha} v_{i\beta} j_\alpha j_\beta)$, coincides with the previously known second-order equilibrium of the ILBM [14]. It should be stressed that while in [4,5] the Maxwellian *must* be truncated to second order (to rescue conservation laws), and thus positivity of populations has to be sacrificed together with the second law of thermodynamics (Boltzmann's H theorem), our Eq. (7) is just a good approximation to the positive equilibrium (6). The discretization of the velocity space done at the level of generating functional (2) violates none of the properties of the continuous kinetic theory [16].

In conclusion, we have derived the genuine lattice Boltzmann model for simulations of incompressible and weakly compressible flows. The new model, unlike the ILBM, is a valid physical model of ideal fluid. It retains the computational efficiency of the ILBM models on the same lattices, and at the same time it extend considerably the domain of validity of simulations especially into the microflow domain. Even in the case of hydrodynamics, the present models should be preferred on the grounds that they correspond more to the physics.

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[1] A. Beskok and G. E. Karniadakis, *Microflows: Fundamentals and Simulation* (Springer, Berlin, 2001).
[2] E. S. Oran, C. K. Oh, and B. Z. Cybyk, Annu. Rev. Fluid Mech. **30**, 403 (1998).
[3] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond* (Oxford University Press, Oxford, 2001).
[4] X. He and L.-S. Luo, Phys. Rev. E **55**, R6333 (1997).
[5] X. Shan and X. He, Phys. Rev. Lett. **80**, 65 (1998).
[6] S. Ansumali, I. V. Karlin, and H. C. Öttinger, Europhys. Lett. **63**, 798 (2003).
[7] S. Ansumali and I. V. Karlin, Phys. Rev. E **66**, 026311 (2002).
[8] X. D. Niu, C. Shu, and Y. Chew, Europhys. Lett. **67**, 600 (2004).
[9] F. Toschi and S. Succi, Europhys. Lett. **69**, 549 (2005).
[10] S. Ansumali, I. V. Karlin, C. E. Frouzakis, and K. B. Boulouchos, Physica (Amsterdam) **359A**, 289 (2006).
[11] S. Ansumali, I. V. Karlin, and H. C. Öttinger, Phys. Rev. Lett. **94**, 080602 (2005).
[12] C. Cercignani, *Theory and Application of the Boltzmann Equation* (Scottish Academic Press, Edinburgh, 1975).
[13] C. Cercignani, M. Lampis, and S. Lorenzani, Phys. Fluids **16**, 3426 (2004).
[14] Y. H. Qian, D. d'Humieres, and P. Lallemand, Europhys. Lett. **17**, 479 (1992).
[15] P. Bassanini, C. Cercignani, and C. D. Pagani, Int. J. Heat Mass Transfer **10**, 447 (1967).
[16] A. N. Gorban and I. V. Karlin, *Invariant Manifolds for Physical and Chemical Kinetics* (Springer, Berlin, 2005).