Consistent Lattice Boltzmann Method

Santosh Ansumali and Iliya V. Karlin

ETH-Zürich, Institute of Energy Technology, CH-8092 Zürich, Switzerland

(Dated: December 21, 2021)

PACS numbers: 05.20.Dd, 47.11.+j

The problem of energy conservation in the lattice Boltzmann method is solved. A novel model with energy conservation is derived from Boltzmann’s kinetic theory. It is demonstrated that the full thermo-hydrodynamics pertinent to the Boltzmann equation is recovered in the domain where variations around the reference temperature are small. Simulation of a Poiseuille micro-flow is performed in a quantitative agreement with exact results for low and moderate Knudsen numbers. The new model extends in a natural way the standard lattice Boltzmann method to a thermodynamically consistent simulation tool for nearly-incompressible flows.

The overwhelming majority of fluid flows of physical and engineering interest are slow. That is, characteristic flow speed $u$ is small compared to the speed of sound $c_s$. This is quantified by the Mach number, $Ma \sim u/c_s$. In typical situations, $Ma$ varies from $10^{-3}$ to $10^{-2}$ in hydrodynamic flows (turbines, reactors etc) to $10^{-4}$ in flows at a micrometer scale. In this paper we address a wide class of flows at $Ma \ll 1$. Then the simplest characterization of the degree of molecularity is the Knudsen number $Kn \sim \lambda/H$, the ratio of the mean free path of molecules $\lambda$ and the characteristic scale $H$ of variation of hydrodynamic fields (density, momentum, and energy). When $Kn \lesssim 10^{-3}$, one considers the hydrodynamic limit where molecularity reduces to specific for each molecular model set of transport coefficients (viscosity, thermal conductivity etc). If, in addition, the Mach number is also small, one enjoys the incompressible hydrodynamics with the ordering $Kn \ll Ma \ll 1$, and the flow can be characterized solely by the ratio $Re \sim Ma/ Kn$ (one of the definitions of the Reynolds number).

Contemporary computational fluid dynamics becomes increasingly more interested in the domain where Mach number remains small but Knudsen number increases, thus, the incompressibility becomes gradually lost. Because of its relevance to the engineering of micro-electromechanical systems (MEMS), the branch of computational fluid dynamics focused on micro scale phenomena is often called “micro-fluidics” [7]. Typical flows in micro-devices are highly subsonic (with characteristic flow velocities about 0.2 $m/s$, corresponding to $Ma \sim 10^{-4}$), while Knudsen number varies from $Kn \sim 10^{-2}$ (so-called slip-flow regime) to $Kn \sim 1$ (moderately rarefied gas flows) [7]. There is much need for computational models in the domain of slow flows where the effects of molecularity become increasingly more pronounced.

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 so-called isothermal lattice Boltzmann models (ILBM) without energy conservation [2]. Recently, there was increasing interest in applying these models also for micro-flow simulations [1 2 4 5 6 8]. The hydrodynamic (locally conserved) fields in the ILBM are the density $\rho$ and the momentum density $j$, whereas the conservation of the energy is not addressed. Construction of the ILBM may vary among the authors, but all these models have one point in common: The lack of energy conservation inevitably leads to a bulk viscosity. Indeed, the non-equilibrium part of the stress tensor in ILBM reads:

$$P_{\alpha\beta}^{neq} \sim Kn \left[ \partial_\alpha \left( \frac{j_\beta}{\rho} \right) + \partial_\beta \left( \frac{j_\alpha}{\rho} \right) \right]. \quad (1)$$

This tensor is not traceless, $P_{\alpha\alpha}^{neq} \sim 2Kn\partial_\alpha(j_\alpha/\rho)$, which immediately leads to the bulk viscosity terms in the equation for the momentum density. We remind 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 non-conservation of the energy. Thus, from the physical standpoint, the bulk viscosity of the ILB models is spurious. 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 $\mathbf{u} = j/\rho$ vanishes in that limit [2]. 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 micro-flow 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 [10] that the flow rate $Q$ has the following asymptotic at low and high Knudsen numbers:

$$Q_0 = (6Kn)^{-1} + s + (2s^2 - 1) Kn, \quad Kn \ll 1$$

$$Q_\infty \sim (1/\sqrt{\pi}) \ln (Kn) + O(1), \quad Kn \to \infty,$$
with \( s = 1.015 \). These two asymptotic limits ensure that the flow rate has a minimum at some finite Kn (the Knudsen minimum [11]). While a qualitative agreement of the ILBM simulations with the continuous-velocity kinetic theory was found at all Knudsen numbers [2,12], the quantitative agreement is poor beyond the slip-flow regime at Kn \( > 10^{-2} \). It was found that the ILBM systematically over-predicts 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 \( \sim \text{Kn} \partial_{\beta} F_{\alpha \beta} \) and the forcing due to the constant pressure gap between the inlet and the outlet. Therefore, if there is additional contribution of the bulk viscosity (more friction), this balance at the same Kn shifts to a higher velocity at the outlet. Therefore, if there is an additional contribution of the bulk viscosity (more friction), this balance at the same Kn shifts to a higher velocity at the outlet, and will result in the over-prediction of the flow rate. On the other hand, the lack of the energy conservation also contributes to the over-prediction at high Knudsen numbers by a different mechanism: Since collisions in the bulk become rare, it becomes important that the energy be correctly redistributed in these rare events.

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

The structure of the paper is as follows: First, we shall derive the discrete-velocity model from the continuous-velocity kinetic theory. Second, we shall redo the computation of the micro-Poiseuille flow with the new model, and demonstrate a significant (roughly, order of magnitude in Kn) improvement in the accuracy with respect to isothermal simulation. Third, we shall explain in which points the present derivation differs from the earlier studies.

A brief discussion concludes the paper.

Starting point of our derivation is the grand canonical potential of the Boltzmann kinetic theory,

\[
H = \int F \ln F d\mathbf{v} + \mu \int F d\mathbf{v} + \zeta_\alpha \int F \rho_{\alpha} d\mathbf{v} + \gamma \int F \mathbf{v}^2 d\mathbf{v},
\]

where \( F(x, v) \) is the one-particle distribution function, and \( \mu, \zeta_\alpha, \) and \( \gamma \) are Langrange 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 \( \rho \), momentum \( j \), and energy \( c \)),

\[
\frac{\partial H}{\partial \mu} = \rho, \quad \frac{\partial H}{\partial \zeta_\alpha} = j_\alpha, \quad \frac{\partial H}{\partial \gamma} = c.
\]

In order to derive the discrete velocity kinetic theory, the functional [2] is evaluated with the help of the \( D \)-dimensional Gauss-Hermite quadrature with the Gaussian weight \( W = (2\pi \theta_0)^{-D/2} \exp \left(-\frac{mv^2}{2\theta_0}\right) \), where \( \theta_0 = (k_B T_0/m) \) is the reduced uniform reference temperature. We remind that the quadrature evaluation of an integral replaces it by a sum, \( \int W(v)G(v) dv \approx \sum_{i=1}^{n_d} W_i G(v_i) \), where \( v_i, i = 1, \ldots, n_d \) are the nodes (or abscissas) of the quadrature, and \( W_i \) are corresponding weights. In the case under consideration, the nodes of the quadrature (discrete velocities) are situated at the zeroes of Hermite polynomials.

We now proceed with the Gauss-Hermite quadrature evaluation of the velocity integral [2]. For concreteness, we shall consider the third-order Hermite polynomial. Then \( n_d = 3D \), and the discrete velocities and weights is constructed as follows: For \( D = 1 \), the three roots and corresponding weights are \( (-\sqrt{3\theta_0}, 0, \sqrt{3\theta_0}) \), \( (1/6, 2/3, 1/6) \); for \( D > 1 \), the roots are all possible tensor roots 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 square lattice which is the crucial feature to the further lattice Boltzmann discretization in space and time. Introducing the populations, \( f_i = W_i (2\pi \theta_0)^{3/2} \exp \left(\frac{v_i^2}{2\theta_0}\right) F(x, v_i) \), and using the reduced discrete velocities, \( c_i = v_i / \sqrt{3\theta_0} \), we write the quadrature for [2]

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

Differentiation of [4] with respect to Lagrange multipliers defines the locally conserved fields in the discrete case (cf. [4]),

\[
\sum_{i=1}^{27} \{1, c_i, c_i^2\} f_i = \{\rho, j_\alpha, 3p + \rho^{-1} j^2\}.
\]

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

\[
f_i^{eq} = W_i \exp \{-\mu - \zeta_\alpha c_i - \gamma c_i^2\}.
\]

In order to express the Lagrange multipliers in [6] in terms of hydrodynamic fields [4], we substitute [4] into [6] and derive the functions \( \mu(\rho, j, p) \), \( \zeta_\alpha(\rho, j, p) \) and \( \gamma(\rho, j, p) \) by perturbation for small momentum, owing for the fact that \( \zeta_\alpha(\rho, 0, p) = 0 \), and that the zero-momentum functions \( \mu(\rho, 0, p) \) and \( \gamma(\rho, 0, p) \) can be found in a closed form. Computation is quite straightforward, and we write here the final result to second order in the momentum:
\[ f_i^\text{eq}(\rho, j, p) = \rho \left( 1 - \frac{p}{\rho} \right)^3 \left( \frac{p}{2 \left( 1 - \frac{p}{\rho} \right)} \right) c_i^2 \left[ 1 + \frac{c_{i\alpha} j_\alpha}{\rho} + \frac{j_\alpha j_\beta}{2 \rho^2} \left( c_{i\alpha} c_{i\beta} - \frac{6E_i^2}{p^2} + \frac{c_i^2 \left( 1 - 3 \frac{p}{\rho} \right) }{3 \left( 1 - \frac{p}{\rho} \right)} \right) \right] . \] (7)

The pre-factor in this formula has the following limit when \( (p/\rho) \to (1/3) \):

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

The implication of this limit will be important below when we will be discussing the relation of the present model to the isothermal lattice Boltzmann model.

We now proceed with the evaluation of the stress tensor \( P_{\alpha\beta}^\text{eq}(\rho, j, p) \) and of the energy flux \( q_\alpha^\text{eq}(\rho, j, p) \) at equilibrium. The important observation to be made here is that if the pressure to density ratio satisfies the condition, then \( P_{\alpha\beta}^\text{eq} \) and \( q_\alpha^\text{eq} \) 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. Moreover, if we allow small variations of the pressure around the point \( p/\rho = 1/3 \), namely, \(|p/\rho - (1/3)| \sim \text{Ma}^2\), the Maxwell’s form of the functions \( P_{\alpha\beta}^\text{eq} \) and \( q_\alpha^\text{eq} \) persists, and we have

\[ P_{\alpha\beta}^\text{eq} = \sum_{i=1}^{27} f_i^\text{eq} c_{i\alpha} c_{i\beta} = p \delta_{\alpha\beta} + j_\alpha j_\beta / \rho, \] (9)

\[ q_\alpha^\text{eq} = \sum_{i=1}^{27} f_i^\text{eq} c_{i\alpha} c_i^2 = \frac{5}{2} j_\alpha j_\alpha / \rho. \] (10)

Note that the variation of the pressure to density ratio of the order \( \text{Ma}^2 \) is pertinent to flow phenomena where the dominant effect on the temperature is the viscous dissipation and associated heat conduction. Condition \(|p/\rho - (1/3)| \sim \text{Ma}^2\) is a conservative estimate of the domain of validity of the present model.

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

\[ \partial_t f_i + c_{i\alpha} \partial_\alpha f_i = -\frac{1}{\tau} (f_i - f_i^\text{eq}(\rho, j, p)), \] (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 \( j_\alpha \) of the order three and higher, and we end up with the following non-equilibrium expressions for the stress and the heat flux:

\[ P_{\alpha\beta}^\text{neq} = -\tau \rho \left[ \partial_\alpha \left( \frac{j_\beta}{\rho} \right) + \partial_\beta \left( \frac{j_\alpha}{\rho} \right) - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma \left( \frac{j_\gamma}{\rho} \right) \right] \] (12)

\[ q_\alpha^\text{neq} = -2 \tau \rho \delta_{\alpha\beta} \left( \frac{p}{\rho} \right) \] (13)

The most important achievement is that the non-equilibrium (Newtonian) stress \( (12) \) is traceless, that is, by preserving the energy conservation we eliminated the spurious bulk viscosity. The heat flux \( (13) \) obeys the Fourier law.

We have implemented the lattice Boltzmann space-time discretization of the kinetic equation \( (11) \), and redo the micro-Poiseuille flow simulation mentioned in the introduction. Results are presented in Fig. 1, where the present model is compared to the exact solution of the continuous linearized BGK model \( (14) \), and the 2DQ9 isothermal lattice Boltzmann model with the spurious bulk viscosity \( (12) \). It is clearly visible that the effect of the spurious bulk viscosity of the isothermal model is completely eliminated, and that the quantitative agreement with the continuous BGK model extends up to \( \text{Kn} = 0.1 \).

![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 \( D2Q9 \) \( (13) \) and the continuous linearized Boltzmann-BGK model \( (14) \).]
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 \( f^{eq}_i \), and use the limit \( \mathbf{5} \), then \( f^{eq}_i(\rho, \mathbf{j}, \rho/3) \) recovers the second-order polynomial equilibrium of the isothermal lattice Boltzmann method on the same lattice\( \mathbf{13, 16} \), and instead of the traceless stress tensor\( \mathbf{12} \) we recover\( \mathbf{11} \) with the bulk viscosity component. It needs to be stressed that the second-order polynomial in\( j \) is an approximation to the positive-definite discrete-velocity equilibrium\( \mathbf{10} \). Same as with the isothermal models, this second-order approximation simply happens to be good enough for stable computations at \( Ma < 0.1 \). If we keep the relation \( p = (1/3)\rho \) to all the orders in\( j \), we recover the exact positive-definite equilibrium of the isothermal 27-velocities entropic lattice Boltzmann model\( \mathbf{13} \):

\[
f^{eq}_i(\rho, \mathbf{j}, \rho/3) = \rho W_i \prod_{\alpha=1}^3 \left( 2 - \sqrt{1 + 3(j_\alpha/\rho)^2} \right) \left( \frac{2 (j_\alpha/\rho) + \sqrt{1 + 3 (j_\alpha/\rho)^2}}{1 - (j_\alpha/\rho)} \right)^{c_{i\alpha}}.
\]

Entropic stabilization procedure\( \mathbf{13, 18, 19} \) can be applied for the present model in order to achieve small values of the transport coefficients but we do not address this here.

Our approach to the discretization of the velocity space differs from the earlier considerations\( \mathbf{20, 21} \). While we use the same Gauss-Hermite quadrature, we apply it on the grand canonical potential\( \mathbf{2} \) (that is, we evaluate the velocity integral\( \mathbf{2} \) as pertinent to the mean of a quadrature), and after that find the discrete-velocity equilibrium upon minimization of the discrete-velocity grand canonical potential\( \mathbf{4} \). Instead, authors of\( \mathbf{20, 21} \) evaluate the local Maxwellian (that is, they evaluate a function, not an integral) of continuous kinetic theory, \( M(\rho, \mathbf{j}, T; \mathbf{v}) = \rho (2\pi k_BT/m)^{-D/2} \exp(-m(\mathbf{v} - \mathbf{u})^2/2k_BT) \), \( \mathbf{4} \), on the nodes of the quadrature. Certainly, just replacing \( M(\rho, \mathbf{j}, T; \mathbf{v}) \rightarrow M_i(\rho, \mathbf{j}, T; \mathbf{v}_i) \) makes no sense because the conservation laws will be lost. However, it was noticed in\( \mathbf{21} \) that when the second-order expansion of the Maxwellian is used instead, \( M^{(2)} = \rho W(1 + av_{i\alpha}j_\alpha + bv_{i\alpha}v_{\beta j_\alpha j_\beta}) \), the replacement, \( M^{(2)} \rightarrow \rho W_i(1 + av_{i\alpha}j_\alpha + bv_{i\alpha}v_{\beta j_\alpha j_\beta}) \), coincides with the previously known second-order equilibrium of the isothermal lattice Boltzmann method\( \mathbf{13, 11} \). It should be stressed that while in\( \mathbf{21, 21} \) the Maxwellian must be truncated to second order (in order to rescue conservation laws), and thus the positivity of populations has to be sacrificed together with the second law of thermodynamics (Boltzmann’s H-theorem), our equation\( \mathbf{7} \) is just a good approximation to the positive equilibrium\( \mathbf{6} \), and, if required, further terms can be computed in order to maintain positivity of the equilibrium populations to any required degree of accuracy. The discretization of the velocity space done at the level of generating functional\( \mathbf{2} \) obviously violates none of the properties of the continuous kinetic theory.

Ref.\( \mathbf{21} \) indicated that the nodes of the fourth-order quadrature can be used for establishing a thermal model. Such model was indeed constructed and implemented in\( \mathbf{13, 22} \). However, even though the admissible temperature variation in this model is larger, it is bound to be less efficient than the lattice Boltzmann method. In that sense, the lattice Boltzmann model with energy conservation derived in this paper is a good compromise for simulations of almost-isothermal low Mach number flows.

In conclusion, we have given a microscopic derivation of a genuine lattice Boltzmann model with energy conservation for simulations of incompressible and almost-incompressible flows. This model is a natural extension of the previously known isothermal models on the same lattices, and, due to the reasons explained above, it was entirely “overlooked” in all previous derivations. While we have considered here the 27-velocities lattice only, we shall address other important cases such as the 15- and 19-velocities 3D lattices and the 9-velocity 2D lattice in our subsequent publications. The new models are as efficient as the previous isothermal lattice Boltzmann models on the same lattices, and at the same time they extend considerably the domain of validity of lattice Boltzmann computations especially into the micro-flow domain. As we have already said, in principle, the spurious bulk viscosity of ILBM is not an obstacle for using them for incompressible hydrodynamics simulation. However, even in that case, the present models can be preferred on the ground that they correspond more to the physics. The approach to the discretization of the microscopic theories uses explicitly the Legendre structure of thermodynamics\( \mathbf{25} \), and can be used in other problems of reducing description. This work was supported by the BFE-Project Nr. 100862.
[1] A. Beskok and G. E. Karniadakis, Microflows: Fundamentals and Simulation (Springer, Berlin, 2001).
[2] S. Succi, The Lattice Boltzmann Equation for Fluid Dynamics and Beyond (Oxford University Press, Oxford, 2001).
[3] S. Ansumali and I. V. Karlin, Phys. Rev. E 66, 026311 (2002).
[4] X. Nie, G. Doolen, and S. Chen, J. Stat. Phys. 107, 279 (2002).
[5] S. Succi, Phys. Rev. Lett. 89, 064502 (2002).
[6] B. Li and D. Kwok, Phys. Rev. Lett. 90, 124502 (2003).
[7] X. D. Niu, C. Shu, and Y. Chew, Europhys. Lett. 67, 600 (2004).
[8] S. Ansumali, I. V. Karlin, C. E. Frouzakis, and K. B. Bouchouchos, Physica A (2005), in press.
[9] S. Ansumali, I. V. Karlin, and H. C. Ottinger, Phys. Rev. Lett. 94, 080602 (2005).
[10] C. Cercignani, Theory and Application of the Boltzmann Equation (Scottish Academic Press, Edinburgh, 1975).
[11] M. Knudsen, Ann. der Physik 28, 75 (1909).
[12] F. Toschi and S. Succi, Europhys. Lett. 69, 549 (2005).
[13] S. Ansumali, I. V. Karlin, and H. C. Ottinger, Europhys. Lett. 63, 798 (2003).
[14] C. Cercignani, M. Lampis, and S. Lorenzani, Phys. Fluid 16, 3426 (2004).
[15] H. Chen, S. Chen, and W. Matthaeus, Phys. Rev. A 45, R5339 (1992).
[16] Y. H. Qian, D. d’Humieres, and P. Lallemand, Europhys. Lett. 17, 479 (1992).
[17] I. V. Karlin, A. Gorban, S. Succi, and V. Boffi, Phys. Rev. Lett. 81, 6 (1998).
[18] I. V. Karlin, A. Ferrante, and H. C. Ottinger, Europhys. Lett. 47, 182 (1999).
[19] B. M. Boghosian, J. Yepez, P. V. Coveney, and A. J. Wagner, Proc. Roy. Soc. Lond. A 457, 717 (2001).
[20] X. He and L.-S. Luo, Phys. Rev. E 55, R6333 (1997).
[21] X. Shan and X. He, Phys. Rev. Lett. 80, 65 (1998).
[22] S. Ansumali, Ph.D. thesis, ETH Zurich, Ref. No. 15534 (2004).
[23] A. N. Gorban and I. V. Karlin, Invariant Manifolds for Physical and Chemical Kinetics (Springer, Berlin, 2005).