A priori derivation of the lattice Boltzmann equation

Xiaoyi He[1,*] and Li-Shi Luo[2,†]

[1]*Center for Nonlinear Studies, MS-B258 and Complex Systems Group (T-13), MS-B213, Theoretical (T) Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*

[2]*ICASE, Mail Stop 403, NASA Langley Research Center, 6 North Dryden Street, Building 1298, Hampton, Virginia 23681-0001*

(Received 21 February 1996)

The lattice Boltzmann equation (LBE) is directly derived from the Boltzmann equation by discretization in both time and phase space. A procedure to systematically derive discrete velocity models is presented. A LBE algorithm with arbitrary mesh grids is proposed and a numerical simulation of the backward-facing step is conducted. The numerical result agrees well with experimental and previous numerical results. Various improvements on the LBE models are discussed, and an explanation of the instability of the existing LBE thermal models is also provided. [S1063-651X(97)51106-8]

PACS number(s): 47.10.+g, 47.11.+j, 05.20.Dd

In the past few years, the lattice Boltzmann equation (LBE) [1–3] has been demonstrated to be an effective computational tool for a broad variety of complex physical systems [4–6] that are problematic for conventional methods. Despite the great interest in the LBE (see, e.g., [4–6]), it has yet to be placed on a rigorous theoretical foundation. This lack of an *a priori* understanding of the LBE has, to a degree, limited its application. For example, calculations based on the LBE have not been very successful in employing arbitrary mesh grids [5,7] and it has not proved possible to satisfactorily simulate thermohydrodynamic systems by means of LBE methods [8–10].

Historically, LBE models evolved from their Boolean counterparts, the lattice-gas automata (LGA) [11,12]. Until now, the theoretical framework of the LBE has rested on the Chapman-Enskog analysis of the LGA models [11,12]. In other words, our understanding of the basis of LBE models has been restricted by our knowledge of the statistical mechanics of LGA.

In this paper, we show that the LBE is a specially discretized form of the continuous Boltzmann equation. Our proof is rigorous and direct and in particular makes no use of the LGA. Thus we establish the LBE on a solid theoretical foundation: the Boltzmann equation. Our argument also has immediate practical consequences. First of all, we make clear how arbitrary mesh grids can be implemented with LBE methods. Second, the Reynolds number accessible in hydrodynamic simulations by LBE methods can now be significantly enhanced. Third, some of the defects in some existing LBE models become apparent from our derivation and we are able to propose improvements with a sound theoretical basis.

For the sake of simplicity and without losing generality, we shall use the Boltzmann Bhatnagar-Gross-Krook (BGK) equation [13,14] in the following analysis. The Boltzmann BGK equation can be written in the form of an ordinary differential equation

$$D_t f + \frac{1}{\lambda} f = \frac{1}{\lambda} g \ , \tag{1}$$

where $D_t \equiv \partial_t + \boldsymbol{\xi} \cdot \boldsymbol{\nabla}$ is the Lagrangian derivative along the microscopic velocity $\boldsymbol{\xi}$, $f \equiv f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ is the single-particle distribution function, λ is the relaxation time due to collision, and g is the Maxwell-Boltzmann distribution function

$$g \equiv \frac{\rho}{(2\pi RT)^{D/2}} \exp\left[- \frac{(\boldsymbol{\xi} - \boldsymbol{u})^2}{2RT} \right], \tag{2}$$

in which R is the ideal gas constant, D is the dimension of the space, and ρ, $\boldsymbol{u}$, and T are the macroscopic density of mass, velocity, and temperature, respectively. The macroscopic variables are the (microscopic velocity) moments of the distribution function f:

$$\rho = \int f \, d\boldsymbol{\xi} \ , \quad \rho \boldsymbol{u} = \int \boldsymbol{\xi} f \, d\boldsymbol{\xi} \ , \quad \rho \varepsilon = \frac{1}{2} \int (\boldsymbol{\xi} - \boldsymbol{u})^2 f \, d\boldsymbol{\xi} \ , \tag{3}$$

where $\varepsilon = D_0 RT/2$ and D_0 is number of the degrees of freedom of a particle.

Equation (1) can be formally integrated over a time interval δ_t:

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \ \boldsymbol{\xi}, \ t + \delta_t) = e^{-\delta_t/\lambda} f(\boldsymbol{x}, \ \boldsymbol{\xi}, \ t) + \frac{1}{\lambda} e^{-\delta_t/\lambda} \times \int_0^{\delta_t} e^{t'/\lambda} \, g(\boldsymbol{x} + \boldsymbol{\xi} t', \ \boldsymbol{\xi}, \ t + t') dt' \ . \tag{4}$$

Assuming that δ_t is small enough and g is smooth enough locally, and neglecting the terms of order δ_t^2 or smaller in the Taylor expansion of the right-hand side of Eq. (4), we obtain

$$f(\boldsymbol{x} + \boldsymbol{\xi}\delta_t, \ \boldsymbol{\xi}, \ t + \delta_t) - f(\boldsymbol{x}, \ \boldsymbol{\xi}, \ t) = -\frac{1}{\tau} [f(\boldsymbol{x}, \ \boldsymbol{\xi}, \ t) - g(\boldsymbol{x}, \ \boldsymbol{\xi}, \ t)] \ , \tag{5}$$

*Electronic address: xyh@t10.lanl.gov

†Electronic address: luo@icase.edu

where $\tau \equiv \lambda/\delta_t$ is the dimensionless relaxation time.

The equilibrium distribution function g can be expanded as a Taylor series in $\boldsymbol{u}$. By retaining the Taylor expansion up to $\boldsymbol{u}^2$, we obtain

$$f^{(\mathrm{eq})} = \frac{\rho}{(2\pi RT)^{D/2}} \exp(-\boldsymbol{\xi}^2/2RT) \times \left\{ 1 + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})}{RT} + \frac{(\boldsymbol{\xi}\cdot\boldsymbol{u})^2}{2(RT)^2} - \frac{\boldsymbol{u}^2}{2RT} \right\} . \quad (6)$$

For the purpose of deriving the Navier-Stokes equations, the above second-order expansion is sufficient.

To derive the Navier-Stokes equations, the following moment integral must be evaluated exactly:

$$\int \boldsymbol{\xi}^m f^{(\mathrm{eq})} d\boldsymbol{\xi} , \quad (7)$$

where $0 \leqslant m \leqslant 3$ for isothermal models and $0 \leqslant m \leqslant 4$ otherwise. The above integral contains the following integral which can be evaluated by Gaussian-type quadrature [15]:

$$I = \int \exp(-\boldsymbol{\xi}^2/2RT)\,\psi(\boldsymbol{\xi})\,d\boldsymbol{\xi} = \sum_\alpha W_\alpha \exp(-\boldsymbol{\xi}_\alpha^2/2RT)\,\psi(\boldsymbol{\xi}_\alpha), \quad (8)$$

where $\psi(\boldsymbol{\xi})$ is a polynomial in $\boldsymbol{\xi}$, and W_α and $\boldsymbol{\xi}_\alpha$ are the weights and the abscissas (or discrete velocities) of the quadrature, respectively. Accordingly, the hydrodynamic moments of Eqs. (3) can be computed by quadrature as well:

$$\rho = \sum_\alpha f_\alpha , \quad \rho \boldsymbol{u} = \sum_\alpha \boldsymbol{\xi}_\alpha f_\alpha , \quad \rho\varepsilon = \frac{1}{2}\sum_\alpha (\boldsymbol{\xi}_\alpha - \boldsymbol{u})^2 f_\alpha , \quad (9)$$

where $f_\alpha \equiv f_\alpha(\boldsymbol{x}, t) \equiv W_\alpha f(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t)$. We shall use the nine-bit isothermal LBE model on square lattice space as a concrete example to illustrate the derivation of LBE models: the evolution equation (5) on a discretized phase space and time, with a proper equilibrium distribution function leading to the Navier-Stokes equations.

To derive the nine-bit LBE model, a Cartesian coordinate system is used and, accordingly, we set $\psi(\boldsymbol{\xi}) = \xi_x^m \xi_y^n$. The integral of Eq. (8) becomes

$$I = (\sqrt{2RT})^{(m+n+2)} I_m I_n , \quad (10)$$

where

$$I_m = \int_{-\infty}^{+\infty} e^{-\zeta^2} \zeta^m \, d\zeta \quad (11)$$

and $\zeta = \xi_x/\sqrt{2RT}$ or $\xi_y/\sqrt{2RT}$. Naturally, the third-order Hermite formula [15] is the optimal choice to evaluate I_m for the purpose of deriving the nine-bit LBE model, i.e., $I_m = \Sigma_{j=1}^3 \omega_j \zeta_j^m$. The three abscissas (ζ_j) and the corresponding weights (ω_j) of the quadrature are

$$\zeta_1 = -\sqrt{3/2} , \quad \zeta_2 = 0 , \quad \zeta_3 = \sqrt{3/2} ,$$
$$\omega_1 = \sqrt{\pi}/6 , \quad \omega_2 = 2\sqrt{\pi}/3 , \quad \omega_3 = \sqrt{\pi}/6 . \quad (12)$$

Then the integral of Eq. (10) becomes

$$I = 2RT \left[\omega_2^2 \psi(\boldsymbol{0}) + \sum_{\alpha=1}^{4} \omega_1\omega_2 \psi(\boldsymbol{\xi}_\alpha) + \sum_{\alpha=5}^{8} \omega_1^2 \psi(\boldsymbol{\xi}_\alpha) \right] , \quad (13)$$

where $\boldsymbol{\xi}_\alpha$ is the zero-velocity vector for $\alpha = 0$, the vectors of $\sqrt{3RT}(\pm 1, 0)$ and $\sqrt{3RT}(0, \pm 1)$ for $\alpha = 1$–4 and the vectors of $\sqrt{3RT}(\pm 1, \pm 1)$ for $\alpha = 5$–8. Note that the above quadrature is exact for $m + n \leqslant 5$.

Now momentum space is discretized with nine discrete velocities $\{\boldsymbol{\xi}_\alpha | \alpha = 0, 1, \ldots, 8\}$. To obtain the nine-bit model, configuration space is discretized accordingly, i.e., it is discretized into a square lattice space with a lattice constance $\delta_x = \sqrt{3RT}\,\delta_t$. It should be stressed that the temperature T has no physical significance here because we are only dealing with an isothermal model. We can therefore choose δ_x to be a fundamental quantity instead, thus $\sqrt{3RT} = c \equiv \delta_x/\delta_t$ or $RT = c_s^2 = c^2/3$, where c_s is the sound speed of the model.

By comparing Eqs. (8) and (13), we can identify the weights defined in Eq. (8):

$$W_\alpha = 2\pi RT \exp(\boldsymbol{\xi}_\alpha^2/2RT)\, w_\alpha , \quad (14)$$

where

$$w_\alpha = \begin{cases} 4/9, & \alpha = 0 \\ 1/9, & \alpha = 1, 2, 3, 4 \\ 1/36, & \alpha = 5, 6, 7, 8. \end{cases} \quad (15)$$

Then the equilibrium distribution function of the nine-bit model is

$$f_\alpha^{(\mathrm{eq})} = W_\alpha f^{(\mathrm{eq})}(\boldsymbol{x}, \boldsymbol{\xi}_\alpha, t) = w_\alpha \rho \left\{ 1 + \frac{3(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})}{c^2} + \frac{9(\boldsymbol{e}_\alpha\cdot\boldsymbol{u})^2}{2c^4} - \frac{3\boldsymbol{u}^2}{2c^2} \right\} , \quad (16)$$

where

$$\boldsymbol{e}_\alpha = \begin{cases} (0, 0), & \alpha = 0 \\ (\cos\theta_\alpha, \sin\theta_\alpha)c, & \alpha = 1, 2, 3, 4 \\ \sqrt{2}(\cos\theta_\alpha, \sin\theta_\alpha)c, & \alpha = 5, 6, 7, 8, \end{cases} \quad (17)$$

and $\theta_\alpha = (\alpha - 1)\pi/2$ for $\alpha = 1$–4 and $(\alpha - 5)\pi/2 + \pi/4$ for $\alpha = 5$–8. Similarly, we can also derive two-dimensional six-bit, seven-bit, and three-dimensional 27-bit LBE models [16].

In the above derivation, the discretization of phase space is accomplished by discretizing momentum space in such a way that a lattice structure in configuration space is simultaneously obtained. That is, the discretization of configuration space is determined by that of momentum space. Of course, the discretization of momentum space and configuration space can be done independently. This consideration has two

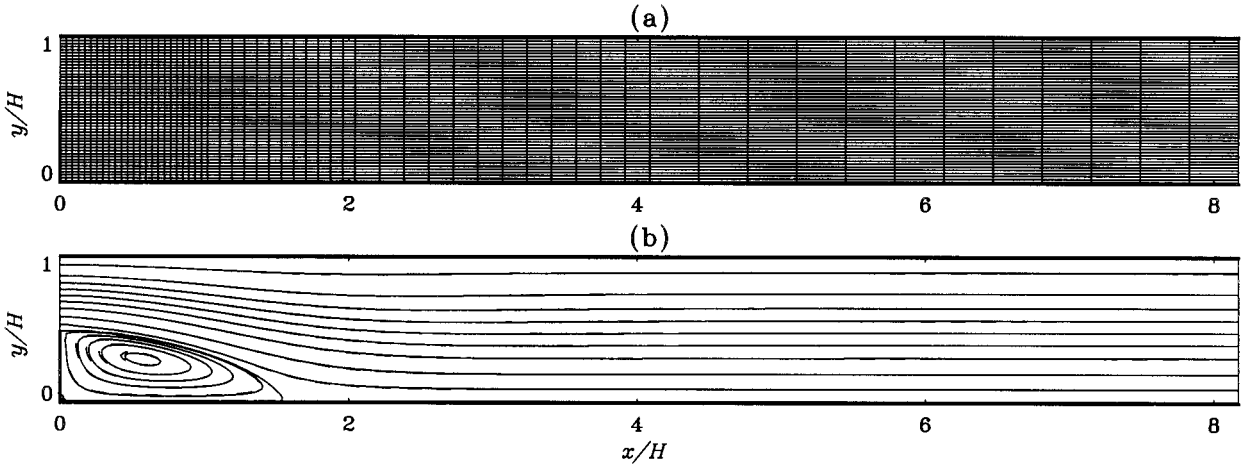

FIG. 1. (a) Nonuniform mesh for the backward-facing step flow simulation. The mesh size is $N_x \times N_y = 61 \times 48$. (b) Streamlines of the backward-facing step flow. The solid lines and dashed lines are the results from the simulations by using the nonuniform mesh and the uniform mesh of size $N_x \times N_y = 385 \times 48$, respectively. The boundary conditions in both simulations are the maximum velocity at entrance $U = 0.1$ and the pressure at the exit $P_1 = 1.0$. The mass density $\rho = 1.0$ and $\tau = 0.596$ in the simulations. The convergence criterion is the relative global difference of the velocity fields (with L^2 norm) between two successive time iterations less than 10^{-7}. In both simulations, the convergence is attained after 50 000 time iterations.

immediate consequences: arbitrary mesh grids and significant enhancement of the Reynolds number in LBE hydrodynamic simulations.

To implement arbitrary mesh grids with the LBE method, one first discretizes the configuration space as one desires for a particular problem, that is, one can first generate a mesh according to the physics of a particular problem. Then, on each grid point, one can discretize momentum space as before. Now a local LBE is built on each mesh grid point. The evolution of this discretized Boltzmann equation (DBE) consists of the following three steps. The first two steps are the usual collision and advection process as in the previous LBE models. After collision and advection, interpolation follows. The interpolation process is what distinguishes the DBE from the LBE method. Because the mesh grids can be arbitrary, the distribution function f_α at one mesh grid point, say $\boldsymbol{X}$, cannot go to another grid point in general through the advection process as it can in previous LBE models. Therefore, the interpolation step becomes necessary to construct $f_\alpha(\boldsymbol{X}, t)$ on each and every mesh grid point from $f_\alpha(\boldsymbol{X} + \boldsymbol{e}_\alpha \delta_t, t)$ after the advection process. Of course, interpolation brings in additional numerical error, but it can be justified as long as the error induced by interpolation does not affect the DBE algorithm as a whole [17]. In addition, the separation of discretizations of momentum space and configuration space allows us to increase the Reynolds number significantly in numerical simulations without enlarging mesh sizes or decreasing the viscosity by adjusting τ [17]. In other words, the limitation posed by the lattice Reynolds number [12,18] is completely overcome and the stability of the LBE method is greatly improved [17].

As an example, we conducted a simulation of the backward-facing step flow [19]. Figure 1(a) illustrates the nonuniform mesh grids used in the simulation. The mesh size is $N_x \times N_y = 61 \times 48$. The geometry of the channel used in our simulation is slightly different from that in Ref. [19] in terms of the ratio between the step height S and the channel height H. ($S/H = 23/47$ in our simulation as opposed to 49/101 in Ref. [19].) A simulation of the flow with a uniform mesh of size $N_x \times N_y = 385 \times 48$ was also conducted. The algorithm used is an improved LBE algorithm for the incompressible Navier-Stokes equation [20], with a second-order upwind interpolation scheme for the nonuniform mesh. The Reynolds number Re of the flow [$\mathrm{Re} = 4U(H-S)/3\nu$ [19], where U is the maximum velocity in the inlet] in our simulation is 100. Figure 1(b) shows the streamlines of both simulations. The difference between the simulations with two meshes, uniform and nonuniform, is hardly visible. The relative global difference (in L^2 norm) of the velocity fields of two simulations is about 0.47%. The location of the reattachment point is $x_1/S = 3.13$ and 3.15 with the uniform and nonuniform meshes, respectively, compared to the experimental measurement of 3.1 in Ref. [19]. This discrepancy of the reattachment location can be attributed to the slight difference in the geometric configuration of the flow.

Another important insight we have gained here is an understanding of the instability of the existing thermal LBE models. We have shown that the equilibrium distribution function $f_\alpha^{(\mathrm{eq})}$ is a special discretized form of the Maxwell-Boltzmann distribution function g and $f_\alpha^{(\mathrm{eq})}$ has a fixed form depending on the details of the discretized velocity set $\{\boldsymbol{\xi}_\alpha\}$. Altering the form of $f_\alpha^{(\mathrm{eq})}$ results in a deviation from the Maxwell-Boltzmann equilibrium, which in turn can affect the stability of the LBE method. Previously, $f_\alpha^{(\mathrm{eq})}$ was obtained by adjusting the coefficients in the polynomial of $\boldsymbol{u}$ such that the Navier-Stokes equation can be derived [21], but the stability constraint was never considered. The scheme seems to work well for the previous LBE isothermal models because the deviation of $f_\alpha^{(\mathrm{eq})}$ from the Maxwell-Boltzmann equilibrium is of order $\boldsymbol{u}^2$. However, the deviation for the thermal models is of order $\boldsymbol{u}$ [9] and it can be fatal. In constructing a correct LBE thermal model, the equilibrium distribution function $f_\alpha^{(\mathrm{eq})}$ is required not only to lead to the Navier-Stokes equations, but also to satisfy the the Maxwell-Boltzmann equilibrium so that the stability of the model is

ensured by the H theorem. Moreover, it is noteworthy that the LBE thermal models are implicit in principle. That means an additional approximation must be introduced.

In conclusion, we have derived the LBE from the Boltzmann equation. The derivation directly connects the LBE to the Boltzmann equation, thus the framework of the LBE can be built on the established foundation of the Boltzmann equation and the rigorous results of the Boltzmann equation can be extended to the LBE. A DBE algorithm with arbitrary mesh has been proposed and validated with the simulation of backward-facing step flow. The algorithm also overcomes the lattice Reynolds number barrier in previous LBE models. In addition, our derivation of the LBE illustrates a systematic and consistent procedure to obtain discrete velocity models from the Boltzmann equation. Finally, an explanation of the instability of the existing LBE thermal models is provided.

X.H. would like to express his gratitude to Dr. Micah Dembo and L.-S.L. to Dr. Gary D. Doolen of LANL for their support and encouragement during this work. L.-S.L. would also like to thank Professor J. Nuttall of University of Western Ontario for helpful discussions on quadrature and orthorgonal polynomials.

[1] G. McNamara and G. Zanetti, Phys. Rev. Lett. **61**, 2332 (1988).

[2] F. J. Higuera, S. Succi, and R. Benzi, Europhys. Lett. **9**, 345 (1989); F. J. Higuera and J. Jeménez, *ibid.* **9**, 663 (1989).

[3] H. Chen, S. Chen, and W. H. Matthaeus, Phys. Rev. A **45**, R5339 (1991); Y. H. Qian, D. d'Humières, and P. Lallemand, Europhys. Lett. **17**, 479 (1992).

[4] *Lattice Gas Methods for Partial Differential Equations*, edited by Gary D. Doolen (Addison-Wesley, Redwood City, CA, 1990); *Lattice Gas Methods: Theory Applications, and Hardware*, edited by Gary D. Doolen (MIT, Cambridge, MA 1991).

[5] R. Benzi, S. Succi, and M. Vergassola , Phys. Rep. **222**, 145 (1992).

[6] J. Stat. Phys. **81** (10) (1995), special issue on lattice-based models and related topics, edited by J. L. Lebowitz, S. A. Orszag, and Y. H. Qian.

[7] S. Succi, G. Amati, and R. Benzi, J. Stat. Phys. **81**, 5 (1995).

[8] F. J. Alexander, S. Chen, and J. D. Sterling, Phys. Rev. E **47**, R2249 (1993).

[9] Y. Chen, H. Ohashi, and M. Akiyama, Phys. Rev. E **50**, 2776 (1994); J. Stat. Phys. **81**, 71 (1995).

[10] G. McNamara, A. L. Garcia, and B. J. Adler, J. Stat. Phys. **81**, 395 (1995).

[11] U. Frisch, B. Hasslacher, and Y. Pomeau Phys. Rev. Lett. **56**, 1505 (1986); S. Wolfram, J. Stat. Phys. **45**, 471 (1986).

[12] U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, Complex Syst. **1**, 649 (1987).

[13] P. L. Bhatnagar, E. P. Gross, and M. Krook, Phys. Rev. **94**, 511 (1954).

[14] R. L. Liboff, *Kinetic Theory* (Prentice-Hall, Englewood Cliffs, N. J., 1990).

[15] P. J. Davis and P. Rabinowitz, *Methods of Numerical Integradion*, 2nd ed. (Academic, New York, 1984).

[16] X. He and L.-S. Luo (unpublished).

[17] X. He and L.-S. Luo, J. Comput. Phys. **129**, 357 (1996).

[18] S. A. Orszag and V. Yakhot, Phys. Rev. Lett. **56**, 1691 (1986).

[19] B. F. Armaly, F. Durst, J. C. F. Pereira, and B. Schönung, J. Fluid Mech. **127**, 473 (1983).

[20] X. He and L.-S. Luo, J. Stat. Phys. (to be published).

[21] G. McNamara and B. J. Adler, Physica A **194**, 218 (1993).